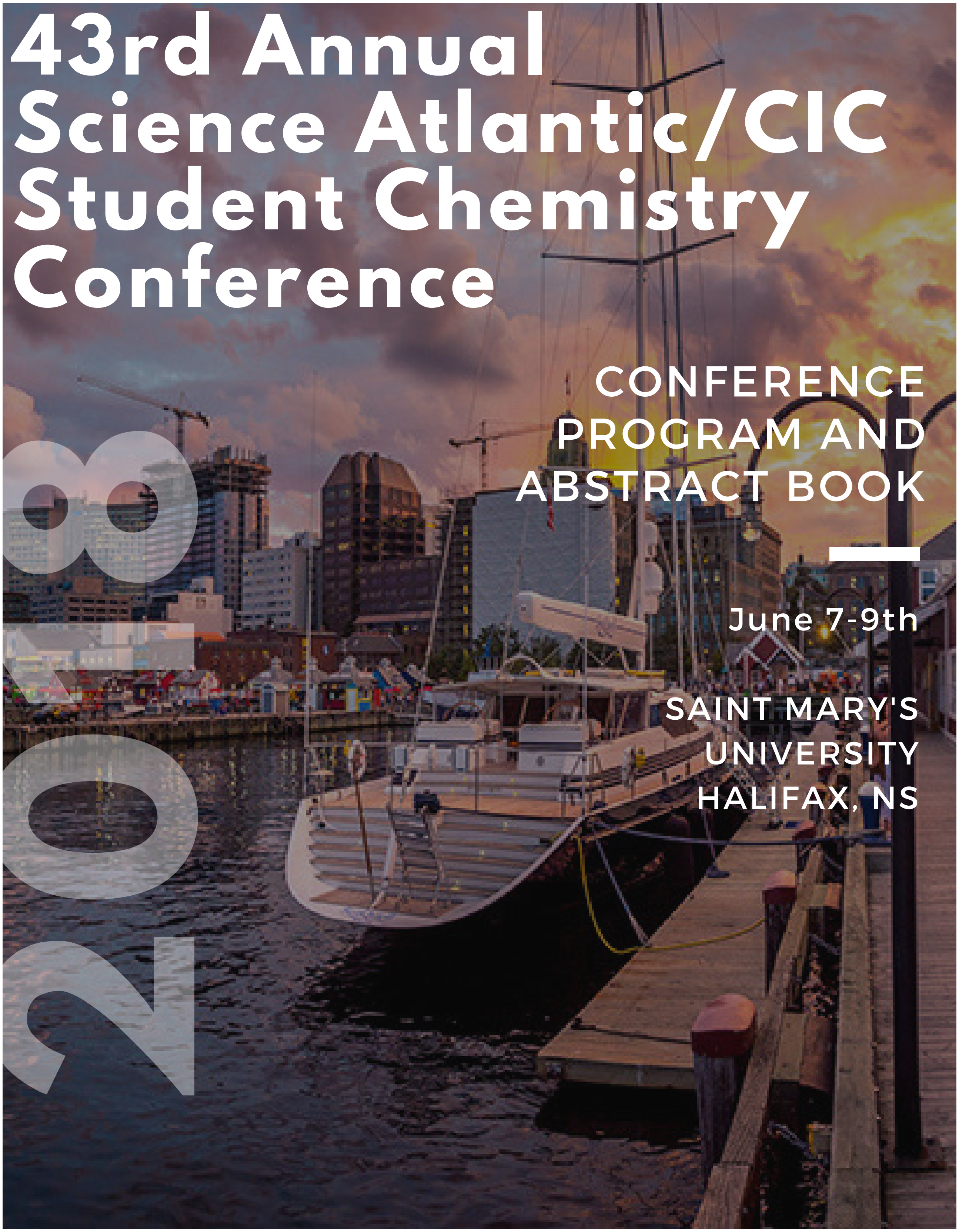
43rd Annual Science Atlantic/CIC Student Chemistry Conference



2018

CONFERENCE PROGRAM AND ABSTRACT BOOK

June 7-9th

SAINT MARY'S
UNIVERSITY
HALIFAX, NS

ChemCon 2018
Going Green

SAINT MARY'S UNIVERSITY SINCE 1802
One University. One World. Yours.

CIC

Science
Atlantic Atlantique

Table of Contents

Sponsors

Gold Level

SMU Chemistry Society
SMU Office of the President
SMU Alumni
SMU Dean of Science
SMU Department of Chemistry
Canadian Society for Chemistry

Silver Level

CIC Organic Division
Canadian Association of Theoretical Chemists (CATC)
BioVectra
CIC Chemistry Education Division
CIC Chemical Education Fund
CIC Maritime Division
The Lord Nelson Hotel & Suites

Bronze Level

CIC Analytical Division
CIC Biological and Medicinal Division
CIC Inorganic Division
CIC Physical, Theoretical, and Computation Division
CIC Materials Division
CIC Newfoundland Division

Sponsors

Bronze Level Continued

Solid State Pharma
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The Crystal Engineering Company®

KRIS TYNSKI
NATURE PHOTOGRAPHER

RE group

FCPC

NSCS

Graduate School & Industry Fair

June 8th from 4:00-6:00 pm

The graduate school & industry fair will take place during the poster session in LA 290.

Graduate School Fair

This fair aims to connect leading institutions with potential students, giving undergraduates and recent graduates the chance to discover future opportunities available to them across Canada. Drop by to speak with representatives, and learn about potential graduate school opportunities at the following universities:

Brock University
Dalhousie University
McGill University
University of New Brunswick
University of Calgary
University of Alberta

Industry Fair

This fair aims to connect chemistry students with industry and organizations from the Atlantic Provinces. Chat with a representative to learn about resources and future opportunities available for chemistry students and graduates from the following businesses and organizations:

BioVectra
Federation of Canada's Professional Chemists (FCPC)
Nova Scotia Chemists Society (NSCS)
National Research Council Canada (NRC)

Campus Map/Parking

Parking for Guests in Accommodation
For guests staying in accommodations on campus, parking is provided at no additional charge. The Arena parking lot is located on the corner of Inglis Street and Tower Road. Please pick up your Parking Pass from the Loyola Front Desk upon arrival and display it in the front windshield of your vehicle.

Parking for Guests not in Accommodation
Passes are $10.00 per day and can be obtained at the Facilities Management Department, Monday to Friday 8:30 AM to 4:30 PM, located on the 1st floor basement of the McNally Building, Room 001 (south side of the building – directly across from the Sobey Building).

Free evening parking is available, Monday to Friday, after 5:00pm in spaces designated as "general" and in "faculty" spaces after 8:00pm. On weekends, all parking spaces can be used. There is no overnight parking permitted.

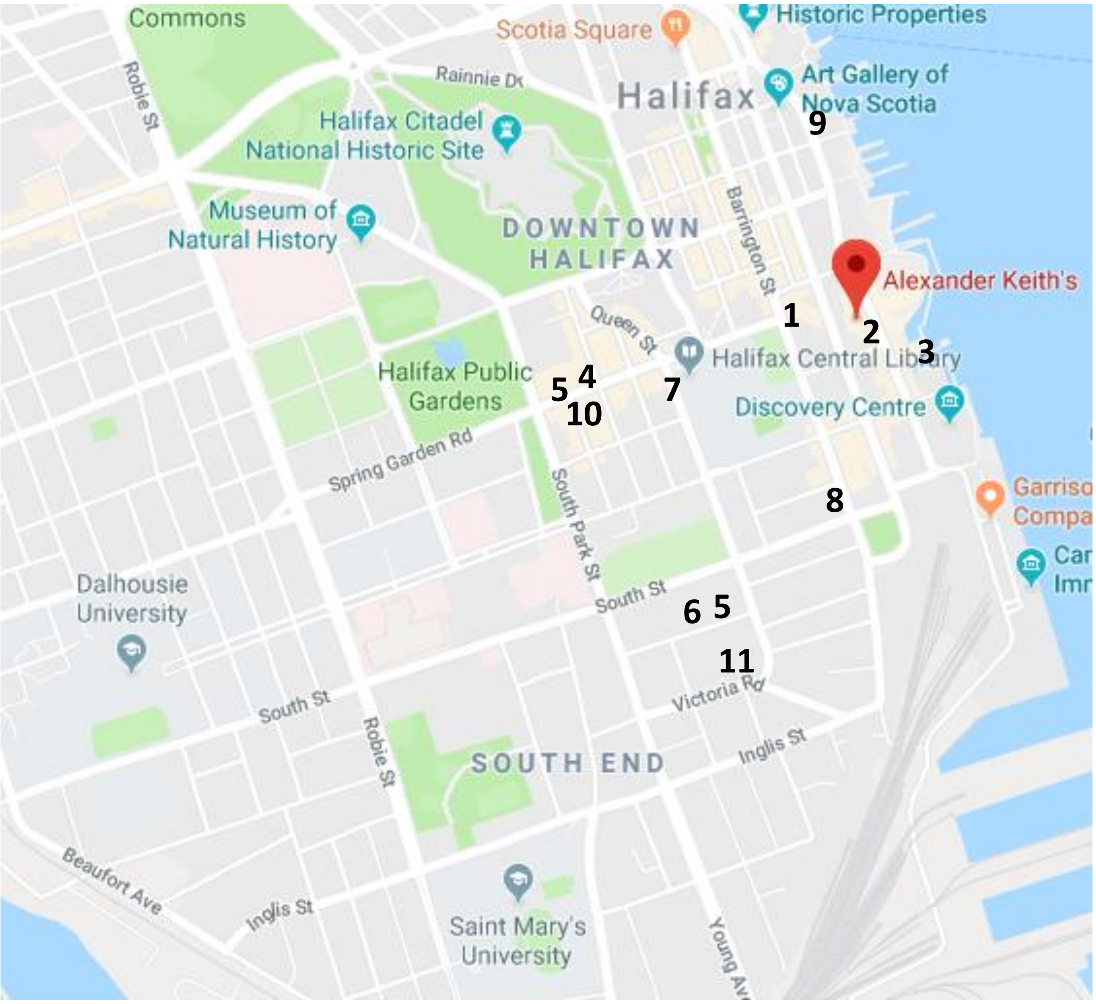
BUILDINGS

AA	Alumni Arena
AG	Art Gallery
AT	Atrium
B	Burke Building
HC	Homburg Centre for Health & Wellness
L	Link Building
LA	Loyola Academic Complex
LR	Loyola Residence
ME	McNally East
MM	McNally Main
MN	McNally North
MS	McNally South
O	The Oaks
PPL	Patrick Power Library
RR	Rice Residence
S	Science Building
SB	Sobey Building
SC	O'Donnell Hennessey Student Centre
VR	Vanier Residence
867	867 Robie St.
883	883 Robie St.
960	960 Tower Rd.
5907	5907 Gorsebrook Ave.
5960	5960 Inglis St.

PARKING

1.	Arena - General, Meters, Accessible
2.	Inglis Street - General, Pay & Display
3.	Science - General, Meters, Faculty, Accessible
4.	McNally East - Meters, Accessible
5.	McNally Main - Faculty, Accessible
6.	Sobey / Gorsebrook - General, Faculty
7.	Oaks - General
8.	Rice - General, Meters, Accessible
9.	Homburg Members Parking Only
10.	Tower Rd - Meters, Accessible

Downtown Halifax



All establishments listed are within 30 minute walking distance from campus.

1. Niche Lounge
2. Red Stag Tavern
3. The Bicycle Thief
4. McDonald's
5. Subway
6. Darrell's Restaurant
7. Sushi Nami
8. Henry House
9. Murphy's Restaurant and Patio
10. Your Father's Moustache/Rock Bottom Brewpub
11. Sobeys/NSLC

List of Awards

CIC Best Overall Oral Presentation in Physical, Theoretical, and Computational Chemistry

CATC Best Overall Oral Presentation in Theoretical Chemistry

CIC Best Overall Poster Presentation in Physical, Theoretical, and Computational Chemistry

CIC Second Best Overall Poster Presentation in Physical, Theoretical, and Computational Chemistry

CATC Best Overall Poster Presentation in Theoretical Chemistry

CIC Best Overall Oral Presentation in Analytical Chemistry

CIC Second Best Overall Oral Presentation in Analytical Chemistry

CIC Best Graduate Poster Presentation in Analytical Chemistry

CIC Best Undergraduate Poster Presentation in Analytical Chemistry

CIC Second Best Undergraduate Poster Presentation in Analytical Chemistry

CIC Best Overall Oral Presentation in Biological and Medicinal Chemistry

CIC Second Best Overall Oral Presentation in Biological and Medicinal Chemistry

CIC Best Overall Poster Presentation in Biological and Medicinal Chemistry

CIC Second Best Overall Poster Presentation in Biological and Medicinal Chemistry

CIC Best Undergraduate Oral Presentation in Materials Chemistry

CIC Best Graduate Oral Presentation in Materials Chemistry

CIC Best Undergraduate Poster Presentation in Materials Chemistry

CIC Best Graduate Poster Presentation in Materials Chemistry

CIC Best Undergraduate Oral Presentation in Inorganic Chemistry

CIC Best Graduate Oral Presentation in Inorganic Chemistry

CIC Best Overall Poster Presentation in Inorganic Chemistry

CIC Second Best Overall Poster Presentation in Inorganic Chemistry

CIC Third Best Overall Poster Presentation in Inorganic Chemistry

CIC Best Undergraduate Oral Presentation in Organic Chemistry

CIC Second Best Undergraduate Oral Presentation in Organic Chemistry

CIC Third Best Undergraduate Oral Presentation in Organic Chemistry

List of Awards

CIC Best Graduate Oral Presentation in Organic Chemistry

CIC Second Best Graduate Oral Presentation in Organic Chemistry

CIC Best Undergraduate Poster Presentation in Organic Chemistry

CIC Second Best Undergraduate Poster Presentation in Organic Chemistry

CIC Best Graduate Poster Presentation in Organic Chemistry

CIC Second Best Graduate Poster Presentation in Organic Chemistry

Science Atlantic Communication Award for Oral Presentations

Science Atlantic Communication Award for Poster Presentations

Science Atlantic Best Overall Undergraduate Research Award for Oral Presentations

Science Atlantic Best Overall Undergraduate Research Award for Poster Presentations

Murray Bruker Award in Chemistry

E. Gordon Young Award

Messages of Welcome

Welcome to the 43rd annual Science Atlantic-CIC Chemistry Conference!

On behalf of Science Atlantic, it is a pleasure to welcome you to the beautiful Saint Mary's campus in Halifax, NS for ChemCon 2018!

Student conferences such as ChemCon provide important opportunities for bright young scientists like you. These student-focused events continue to improve with each passing year, providing high-quality, professional venues for science students to share their research, be inspired by fascinating keynote speakers, and get to know others who share your interests and passion for science.

Whether it's gaining feedback on your presentation, learning about the exceptional research taking place in our region, or meeting your future supervisor or employer, you will be provided with valuable opportunities this weekend that may help you determine the next step in your scientific career.

Your conference organizers and volunteers have worked hard to make this year's ChemCon a great event. Please take a moment during the conference to show them your appreciation; it wouldn't have happened without them!

Enjoy the conference!

Sincerely,

L Whitehead

Lois Whitehead

Executive Director, Science Atlantic

Messages of Welcome

Dear Undergraduates, Graduate Students, and Colleagues,

On behalf of the Faculty of Science at Saint Mary's University, it is my pleasure to welcome you to ChemCon, the 2018 Science Atlantic Chemistry Conference. Our ChemCon team has worked hard to pull together an impressive program featuring keynote speakers, student talks, discussion panels, an industry fair, and entertainment, and I hope you'll find value in the entire schedule.

Every year ChemCon is an amazing opportunity for you to talk about science with experts from across Canada, and I encourage you to ask questions – lots of questions! These industry experts, faculty members and graduate students have been in your shoes and they have the answers about your future education and career goals.

This is a great opportunity to make key connections and practice communicating about your work, two skills that are vital in both education and the workforce. Our faculty members are pros at speaking to the public about their research, and have learned how to explain complex topics in an accessible way, on TV, on the web, and on social media.

Good luck with your presentations, I look forward to hearing about your work. It is inspiring to hear about the great work happening at universities in Atlantic Canada.

We are thrilled to have you here visiting us in Halifax. Enjoy your time on campus and we hope you will also appreciate what the city has to offer.

Sincerely,

Dr. Steven Smith

Dean of Science, Saint Mary's University

Conference Organizing Committee

Conference Chair
Taylor Lynk

Treasurer
Melanie Davidson

Fundraising Coordinator
Kaitlyn Blatt-Janmaat

Food and Venue Coordinator
Rafee Hossain

Guest Speaker and Volunteer Coordinator
Jennifer Wright

Webmaster
Jason d'Eon

Judging and Awards Coordinator
Chandika Ramful

Graduate Fair/Trade Show Coordinator
Navya Kesavan

Faculty Supervisor
Dr. Kai Ylijoki

List of Student Presenters

Acadia University

Angela Kaiser
Anderson Fuller
Miranda Walsh
Katharine Miller
Mimoza Gjelaj
Mollie MacLean
Jenny Gao-Kang
Jenna McNutt
Jun Luo

Cape Breton University

Haley Armstrong
Shanghua Feng

Dalhousie University

Erin Welsh
Dylan Hale
Chris Lavoie
Shayne Gracious
Toren Hynes
Ryan McGuire
David Hall
Blake Huchenski
Aaron Liu
Min Joon Kim
Casper Macaulay
Sarah Greening
Luke Murphy
Lauren Thompson
Helia Hollenhorst
Leah Ellis
Philip Jakubec
Tyler van de Ven
Efthimios Karmas
Alana Rangaswamy
Roberto Diaz-Rodriguez
Govinda Humagain
Yiqi Lai
Maxine Kirshenbaum
Melody Yue Shen
Alexander Hare
Felicia Licht
David Morris
Alastair Price
Sarah Greening
Fabien Lindeperg

Memorial University of Newfoundland

Laurie Donnelly
Matthew Johnson
Kelsey Menard
Archita Adluri
Victoria Rose
Courtney Laprise
Holly Barrett
Juliana Vidal
Christopher Qiu

Mount Allison University

Andrew Linton
Adam Beckett
Meagan Kindervater
Marcus Kindervater
Sarah Martell
Kathleen Morrison
Maia Murphy
Isabel Curtis
Katherine Reiss
Max Landry

List of Student Presenters

Mount Saint Vincent University

Yuriy Barchuk
Guilherme Ferreira
Kosuke Kanayama

Queen’s University

Caroline Spence-Elder

Saint Mary’s University

Chandika Ramful
Katrina Turrie
Ernlie Publicover
Kaitlyn Blatt-Janmaat
Jennifer Kolwich
Katherine Parsons
Robert Riley
Taylor Lynk
Melanie Davidson
Najwan Albarghouthi
Michael Land
Matthew Laprade
Mary Laeticia Wendy Rose
Ariana Joseph
Shruti Bindesri
Kathleen Allen
Gaius St. Marie
Morgan Crosby
Ketnavi Ramgoolam
Jennifer Wright
Kalei Crowell
Ryan Hines
Ryan McCoy
Katherine Budden
Ian Desmond Conrod
Brendan Grue

St. Francis Xavier University

Andrew Duffy
Bry Crabbe
Pablo Scrosati
Katie Doran

Université de Moncton

Alexandre LeBlanc
Ben Yaala Hamza
Abdou Ben Ali Adluri
Ndongou-Moutombi Fanta

University of New Brunswick

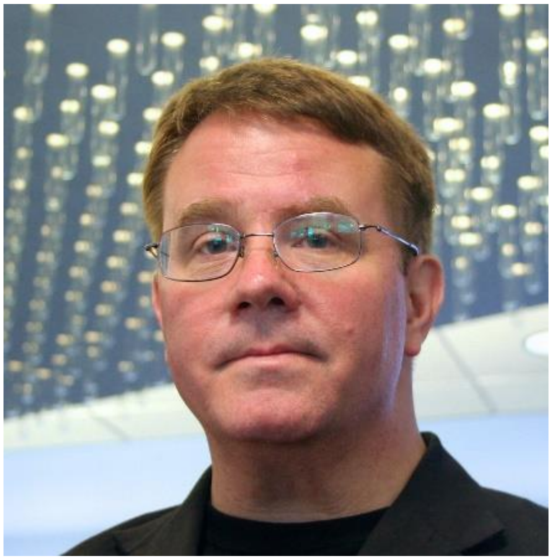
Brandon Frenette
Genesis Infante
Brandon Fillmore
Nigel Patterson
Morgan Burgoyne
Steven McWilliams
Amar Kumar Bhardwaj
Livia Ferland
Sydney Hetherington
Amy Brown
Jayden Price

University of Toronto

Tam Pham

Keynote Speakers

Dr. John Warner

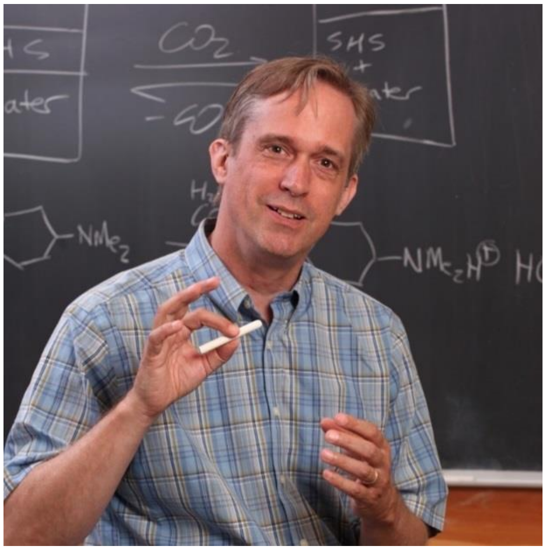


Dr. John Warner is the recipient of the 2014 Perkin Medal and is widely acknowledged as the highest honour in American Industrial Chemistry. He was also named a 2016 AAAS-Lemelson Invention Ambassador. Dr. Warner received his BS in Chemistry from UMASS Boston and his PhD in chemistry from Princeton University. After working for the Polaroid Corporation he served as tenured full professor at UMASS Boston and Lowell. In 2007 he founded the Warner Babcock Institute for Green Chemistry, LLC (a research organization developing green chemistry technologies) where he serves as President and Chief Technology Officer, and Beyond Benign (a non-profit dedicated to sustainability and green chemistry education). Dr. Warner is one of the founders of the field of Green Chemistry. He has published nearly 300 patents, papers and books. Dr. Warner received the 2004 Presidential Award for Excellence in Science Mentoring, the American Institute of Chemistry’s Northeast Division Distinguished Chemist of the Year for 2002 and the Council of Science Society President’s 2008 Leadership award. He was named by ICIS as one of the most influential people impacting the global chemical industries, In 2011 he was elected a fellow of the American Chemical Society and names one of the “25 Visionaries changing the World” by Utne Reader.

June 7th from 5:40 pm - 6:40 pm in McNally Main Auditorium

Keynote Speakers

Dr. Philip Jessop



Dr. Philip Jessop is the Canada Research Chair of Green Chemistry at Queen’s University and the Technical Director of GreenCentre Canada. After his Ph.D. (UBC, 1991) and a postdoctoral appointment (Toronto, 1992), he did contract research in Japan with Ryoji Noyori (Nobel Prize 2001). As a professor at the University of California-Davis (1996-2003) and since then at Queen’s, Jessop has studied green solvents and the chemistry of CO_2. Distinctions include the Eni Award for New Frontiers for Hydrocarbons (2013), Fellowship in the Royal Society of Canada (2013), the Canadian Green Chemistry & Engineering Award (2012), and the NSERC Polanyi Award (2008). He serves as Chair of the Editorial Board for the journal *Green Chemistry*, has chaired two international conferences and helped create GreenCentre Canada, a National Centre of Excellence for the commercialization of green chemistry technologies. His inventions include switchable solvents, more environmentally-friendly paints, and a low-energy method for purifying wastewater. Switchable Solutions Inc. and Forward Water Technologies Inc. are spin-off companies based upon Dr. Jessop's technologies.

June 8th from 1:15 pm - 2:15 pm in McNally Main Auditorium

Discussion Panels

June 8th from 12:30-1:30 pm

Choose a discussion panel to attend during lunch (boxed lunches will be provided).

Women in STEM

with Stephanie MacQuarrie, Christa Brosseau, and Clarissa Sit

Join a discussion about notable women in chemistry and being a woman in a male-dominated industry. This discussion panels aims to spark an open discussion about systematic challenges faced by women in STEM, and how male advocates, managers, and educators can help to address these challenges.

Green Chemistry

with Philip Jessop, Jason Clyburne, and Leah Ellis

Join a discussion about how to become more involved in the sustainable advancement of chemistry. This discussion panel will address both the advantages and challenges associated with practicing green chemistry.

Employment in Chemistry

with Laura Reyes, Stephen DeGrace, and Danielle Tokarz

Join a discussion about what jobs exist for chemistry graduates in both industry and academia, and how to best prepare yourself to gain employment in the STEM field.

Schedule of Events

Thursday, June 7th

11:00 am - 2:45 pm Registration in *McNally Main Lobby*
Visit us at the registration table to check in and get your name tag, event tickets, and important information regarding the conference. Registration is mandatory for all conference attendees. If you can't make it during this time, let us know and we will set something up!

2:45 pm - 3:15 pm Opening remarks in *McNally Main Auditorium*
Opening remarks by SMU Vice President Dr. Malcom Butler, Conference Co-Chair Taylor Lynk, and CIC representative Laura Reyes.

3:15 pm - 5:30 pm Student Talks Session 1 in *McNally Main Auditorium* (with break at 4:15)
Oral Presentations by undergraduate and graduate students in the fields of organic and inorganic chemistry.

5:40 pm - 6:40 pm Dr. John Warner, Keynote Speaker in *McNally Main Auditorium*

6:45 pm - 7:30 pm Pizza Dinner at the *Gorsebrook*
You must be 19 years of age or older to attend this event. Canadian government issues ID is required for entry.

7:30 pm - 12:00 am Trivia and Mixer at the *Gorsebrook*
Come play some trivia, maybe win some great prizes, and meet your fellow conference attendees. You must be 19 years of age or older to attend this event. Canadian government issued ID is required for entry.

Friday, June 8th

6:30 am - 7:30 am Morning run at *Point Pleasant Park*
Meet in front of the Homburg Center (SMU gym) to take a group run, walk, or jog around Point Pleasant Park. Weather permitting.

7:30 am - 8:10 am Breakfast at the *Dockside Dining Hall*
Breakfast is included only for those staying in SMU residence. The cost of breakfast is $8.25 for those staying off campus. There is also a Tim Hortons on campus in the Loyola Academic building.

8:15 am - 10:00 am Student Talks Session 2 in *McNally Main Auditorium*
Oral presentations by undergraduate students in the fields of materials and organic chemistry.

10:00 am - 10:15 am Nutritional Break in *McNally Main Lobby*

Schedule of Events

10:15 am - 11:45 am Student Talks Session 3 in *McNally Main Auditorium*
Oral presentations by undergraduate students in the fields of biological and medicinal chemistry and physical, theoretical, and computational chemistry.

11:45 am - 12:00 pm Lunch in *McNally Main Lobby*
Grab a boxed lunch before heading to one of the discussion panels.

12:00 pm - 1:00 pm Discussion Panels in *Sobey Building Classrooms*
There are three panels offered over lunch: Women in STEM, Green Chemistry, and Employment in Chemistry.

1:15 pm - 2:15 pm Dr. Philip Jessop, Keynote Speaker in *McNally Main Auditorium*

2:30 pm - 4:00 pm Student Talks Session 4 in *McNally Main Auditorium*
Oral presentations by undergraduate students in the fields of organic and inorganic chemistry.

3:30 pm - 4:00 pm Poster set up in *Loyola Conference Hall*
You may set up your poster during this time, of you can drop your poster off to a conference organizer/volunteer at any time during the day and we will set it up for you so you don't miss any conference activities. There will be a poster drop-off area in the McNally Main Lobby.

4:00 pm - 6:00 pm Poster Session/Grad School & Industry Fair in *Loyola Conference Hall*
Poster presentations by undergraduate and graduate students in all fields of chemistry. Chat with a graduate school or industry representative about your future opportunities in chemistry, this event is all about networking. Refreshments will be provided.

6:00 pm – 7:00 pm Science Atlantic Meeting in *Sobey Building Room 159*

7:00 pm – 8:00 pm CIC Maritime Division Meeting in *Sobey Building Room 159*

8:30 pm - 9:00 pm Group walk to Keith's Brewery from the *Student Union Building*
Meet outside the Student Union Building to walk to Alexander Keith's Brewery. If it is raining we will provide bus tickets. You can also meet us at Keith's if you will be off campus beforehand getting supper.

9:00 pm - 11:00 pm *Keith's Brewery Tour* (guided walk leaving from SMU at 8:30)
Learn about the history of Alexander Keith's Brewery, socialize, and enjoy some live music and complementary beverages. Snacks will be provided. ***This is an all ages event*** (underage attendees will not be served alcohol).
If you are returning back to SMU after this event we will be walking back as a group as well. If you choose to stay downtown you are responsible for getting back to campus.

Schedule of Events

Saturday, June 9th

7:30 am - 8:45 am Breakfast at the *Dockside Dining Hall*
Breakfast is included only for those staying in SMU residence. The cost of breakfast is $8.25 for those staying off campus. There is also a Tim Hortons on campus in the Loyola Academic building.

9:00 am - 10:30 am Student Talks Session 5 in *McNally Main Auditorium*
Oral presentations by undergraduate and graduate students in the fields of analytical, biological and medicinal and physical, theoretical and computational chemistry.

10:30 am - 10:45 am Nutritional break in *McNally Main Lobby*

10:45 am - 12:15 pm Student Talks Session 6 in *McNally Main Auditorium*
Oral presentations by graduate students in the fields of materials and organic chemistry.

12:30 pm - 1:30 pm Lunch at the *Dockside Dining Hall*
Lunch is included for all attendees. Your meal hall ticket will be included in your welcome package.

1:45 pm - 3:15 pm Student Talks Session 7 in *McNally Main Auditorium*
Oral presentations by graduate students in the fields of inorganic and organic chemistry.

3:15 pm - 3:30 pm Nutritional Break in *McNally Lobby*

3:30 pm – 5:00 pm Student Talks Session 8 in *McNally Main Auditorium*
Oral presentations by graduate students in the fields of materials and inorganic chemistry.

5:15 pm - 6:15 pm Judges Meeting in *Sobey 159*

6:45 pm - 7:30 pm Cocktails **(Banquet)** in *Loyola Conference Hall*
To attend banquet events, you must purchase a banquet ticket before the conference.

7:30 pm - 8:30 pm Dinner **(Banquet)** in *Loyola Conference Hall*
To attend banquet events, you must purchase a banquet ticket before the conference.

8:30 pm - 8:50 pm Science Atlantic Pin Presentations in *Loyola Conference Hall*

8:50 pm - 9:30 pm Awards Ceremony in *Loyola Conference Hall*

9:30 pm - 10:00 pm Bids for ChemCon 2020 in *Loyola Conference Hall*

Oral Presentation Schedule

Thursday, June 7th 2018

Session 1

Time	Speaker	School	Division
3:15 pm – 3:30 pm	Angela Kaiser	Acadia	Organic
3:30 pm – 3:45 pm	Brandon Frenette	UNB (Fredericton)	Inorganic
3:45 pm – 4:00 pm	Chandika Devi Ramful	SMU	Organic
4:00 pm – 4:15 pm	Katrina Turrie	SMU	Inorganic
4:30 pm – 4:45 pm	Erin Welsh	Dalhousie	Organic
4:45 pm – 5:00 pm	Dylan Hale	Dalhousie	Inorganic
5:00 pm – 5:15 pm	Caroline Spence-Elder	Queen’s	Organic
5:15 pm – 5:30 pm	Chris Lavoie	Dalhousie	Inorganic (Grad)

Friday, June 8th 2018

Session 2

Time	Speaker	School	Division
8:15 am – 8:30 am	Andrew Linton	Mount Allison	Materials
8:30 am – 8:45 am	Ernlie Publicover	SMU	Organic
8:45 am – 9:00 am	Laurie Donnelly	MUN	Materials
9:00 am – 9:15 am	Haley Armstrong	CBU	Organic
9:15 am – 9:30 am	Shayne Gracious	Dalhousie	Material
9:30 am – 9:45 am	Matthew Johnson	MUN	Organic
9:45 am – 10:00 am	Andrew Duffy	StFX	Organic

Oral Presentation Schedule

Session 3

Time	Speaker	School	Division
10:15 am – 10:30 am	Kelsey Menard	MUN	Phys., Theor., & Comp.
10:30 am – 10:45 am	Kaitlyn Blatt-Janmaat	SMU	Biological/Medicinal
10:45 am – 11:00 am	Anderson Fuller	Acadia	Phys., Theor., & Comp.
11:00 am – 11:15 am	Tam Pham	UofT	Biological/Medicinal
11:15 am – 11:30 am	Archita Adluri	MUN	Phys., Theor., & Comp.
11:30 am – 11:45 am	Jennifer Kolwich	SMU	Biological/Medicinal

Session 4

Time	Speaker	School	Division
2:30 pm – 2:45 pm	Toren Hynes	Dalhousie	Organic
2:45 pm – 3:00 pm	Katherine Parsons	SMU	Organic
3:00 pm – 3:15 pm	Ryan McGuire	Dalhousie	Inorganic
3:15 pm – 3:30 pm	Miranda Walsh	Acadia	Organic
3:30 pm – 3:45 pm	Victoria Rose	MUN	Organic
3:45 pm – 4:00 pm	Robert Riley	SMU	Inorganic

Saturday, June 9th 2018

Session 5

Time	Speaker	School	Division
9:00 am – 9:15 am	Taylor Lynk	SMU	Analytical
9:15 am – 9:30 am	David Hall	Dalhousie	Phys., Theor., & Comp. (Grad)
9:30 am – 9:45 am	Melanie Davidson	SMU	Analytical (Grad)
9:45 am – 10:00 am	Alexandre Leblanc	UdeM	Biological/Medicinal (Grad)
10:00 am – 10:15 am	Hamza Ben Yaala	UdeM	Analytical (Grad)
10:15 am – 10:30 am	Najwan Albarghouthi	SMU	Analytical (Grad)

Oral Presentation Schedule

Session 6

Time	Speaker	School	Division
10:45 am – 11:00 am	Bry Crabbe	StFX	Materials (Grad)
11:00 am – 11:15 am	Blake Huchenski	Dalhousie	Organic (Grad)
11:15 am – 11:30 am	Courtney Laprise	MUN	Materials (Grad)
11:30 am – 11:45 am	Michael Land	SMU	Organic (Grad)
11:45 am – 12:00 pm	Aaron Liu	Dalhousie	Materials (Grad)
12:00 pm – 12:15 pm	Min Joon Kim	Dalhousie	Organic (Grad)

Session 7

Time	Speaker	School	Division
1:45 pm – 2:00 pm	Casper Macaulay	Dalhousie	Inorganic (Grad)
2:00 pm – 2:15 pm	Genesis Infante	UNB (Fredericton)	Organic (Grad)
2:15 pm – 2:30 pm	Matthew Laprade	SMU	Inorganic (Grad)
2:30 pm – 2:45 pm	Sarah Greening	Dalhousie	Organic (Grad)
2:45 pm – 3:00 pm	Luke Murphy	Dalhousie	Inorganic (Grad)
3:00 pm – 3:15 pm	Brandon Fillmore	UNB (Fredericton)	Organic (Grad)

Session 8

Time	Speaker	School	Division
3:30 pm – 3:45 pm	Lauren Thompson	Dalhousie	Materials (Grad)
3:45 pm – 4:00 pm	Helia Hollenhorst	Dalhousie	Inorganic (Grad)
4:00 pm – 4:15 pm	Nigel Patterson	UNB (Fredericton)	Materials (Grad)
4:15 pm – 4:30 pm	Morgan Burgoyne	UNB (Fredericton)	Inorganic (Grad)
4:30 pm – 4:45 pm	Leah Ellis	Dalhousie	Materials (Grad)
4:45 pm – 5:00 pm	Steven McWilliams	UNB (Fredericton)	Inorganic (Grad)

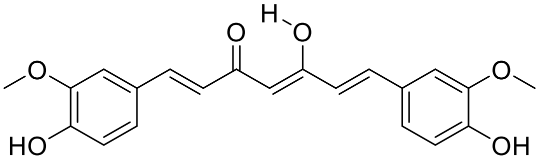
Carbocyclic analogs of curcumin as neuroprotecting agents

Angela Kaiser[1], Brian Wilson[1], Dani Youssef[2], and Amitabh Jha[1]

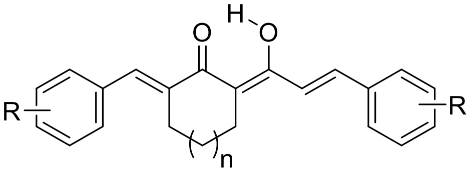
[1]Acadia University
[2]Université Sainte-Anne

Division: Undergraduate Organic

Curcumin is a phytochemical obtained from turmeric, a heavily consumed spice in Indian subcontinent. The significant health benefits demonstrated by curcumin in-vitro is marred by its poor bioavailability in-vivo. In an attempt to overcome this challenge, we have prepared cyclic analogues retaining the curcumin pharmacophore. We developed an expeditious synthesis of these compounds which involves the condensation of 2-acetylcycloalkanones with various aromatic aldehydes to form 2-arylidene-6-(3-arylacryloyl)cycloalkanones derivatives. Curcumin is known to possess antioxidant properties and as such, represents a potential stroke therapeutic. Increased production of free radicals associated with ischemic stroke exacerbates brain damage by inducing neuronal apoptosis. It was thought that these curcumin analogs would reduce cell death in hypoxic organotypic brain slice cultures by mitigating free radical tissue damage. Results obtained thus far will be presented.



Curcumin



Carbocyclic curcumin analogs

Toward a Series of New Tetra(iminophosphorano)-Substituted Bispyridinylidene Organic Electron Donors

Brandon Frenette, Adam Dyker, and Nadine Arseneault

University of New Brunswick

Division: Undergraduate Inorganic

A series of new ground state organic electron donors featuring four strongly π-donating iminophosphorano (-N=PR3) substituents on a bispyridinylidene skeleton has been explored. These new donors improve upon the previously reported strongest organic reducing agent, a tetrakis(triphenyliminophosphorano)-substituted bispyridinylidene,1 via changing to more strongly π-donating tricyclohexyliminophosphorano substituents. This change of substituents should result in a more negative reduction potential, proportional to the π-donation ability of the substituent. Through systemically replacing the triphenyliminophosphorano substituents with tricyclohexyliminophosphorano groups at the ortho, para, and both positions, three new organic reducing agents could be envisaged. This series of bispyridinylidenes represents the most powerful neutral organic electron donors ever reported and should be capable of expanding the scope of reductions which can be carried out by organic molecules.

1. Hanson, S. S.; Doni, E.; Traboulsee, K. T.; Coulthard, G.; Murphy, J. A.; Dyker, C. A. Angew. Chem. Int. Ed. 2015, 54, 11236–11239.

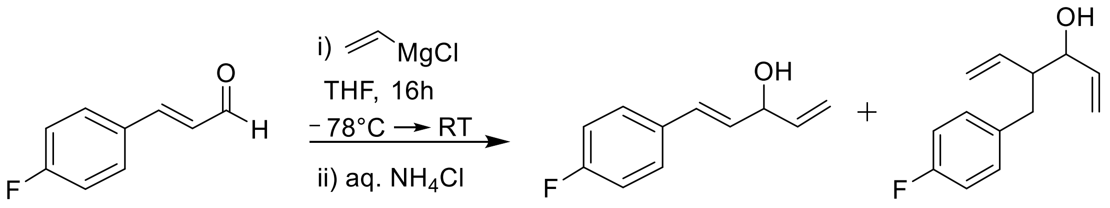
Exploration of diastereoselective double alkylation reactions of Grignard reagents with cinnamaldehydes

Chandika D. Ramful, Kalei Crowell, and Kai E.O. Ylijoki*

Saint Mary's University

Division: Undergraduate Organic

We have recently observed a novel reaction of a Grignard reagent with 4-fluorocinnamaldehyde. We propose that the reaction results in a diastereoselesctive double alkylation, leading to two predominant products as indicated by NMR spectroscopy and column chromatography (Scheme 1). The proposed double alkylated product has been characterized. Such a reaction triggers great synthetic interest and is also intriguing from a mechanistic perspective. Our group is now focusing on optimizing the reaction conditions and expanding the scope of the reaction to other Grignard reagents and cinnamaldehydes combinations. Crystallization will be conducted to characterize the products by X-ray crystallography to determine which diastereomer is being produced.



Simple Polyhalide Salts of the Dimethylammonium Cation

Katrina D. Turrie, Jason A. C. Clyburne, Michael A. Land, and Katherine N. Robertson

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Division: Undergraduate Inorganic

A novel $[(Me)_2NH_2]_2$ $[I_2Cl_2]$ complex was isolated and characterised using X-ray crystallography. The crystal structure of the dianion, [Cl---I—I---Cl], contains both covalent bonds between the central I_2 atoms and halogen-halogen contact bonds between the outer Cl atoms and the diatomic I_2 center. This anion has only been reported a number of times and with more complex cations, however, our results show that large cations are not needed for stabilization.[1] Robertson *et al.*, have previously reported salts of the dimethylammonium cation with both the I^- and I_3^- anions.[2] In this investigation we have prepared two additional compounds which have been isolated and characterised, $[(Me)_2NH_2]_2$ $[I_3]$ [Cl] and $[(Me)_2NH_2]$ $[ICl_2]$. Given the variety of the anions isolated, our reported salts have the potential to be widely applicable in a number of different technological sectors such as dye sensitized solar cells and electrolytes in batteries.[3]

1. Marti-Rujas J.; Meazza L.; Lim G. K.; Terraneo G.; Pilati T.; Harris K. D. M.; Metrangolo P.; Resnati. G. *Angew. Chem.*, *Int. Ed.*, 2013 **52,** 13444. Parigoridi I.-E.; Corban G. J.; Hadjikakou, S. K.; Hadjiliadis, N.; Kourkoumelis, N.; Kostakis, G.; Psycharis, V.; Raptopoulou, C. P.; Kubicki, M. *Dalton Trans.* 2008,**0**,5159-5165.

2. Robertson, K. N.; Cameron, T.; Knop, O. *Can. J. Chem.* 1996, **74,** 1572-1591.

3. Gorlov, M.; Pettersson, H.; Hagfeldt, A.; Kloo, L. *Inorg. Chem.* 2007, **46,** 3566-3575. Weng, G.; Li, Z.; Cong, G.; Zhou, Y.; Lu, Y. *Energy Environ. Sci.* 2017, **10,**735-741.

Second Generation Chiral Diazaphospholenes

Erin Welsh and Dr. Alex Speed

Dalhousie University

Division: Undergraduate Organic

The metal-free catalytic reduction of unsaturated molecules is an emerging field of chemistry. Well-established transition metal-catalyzed reductions are efficient, and highly selective in many cases. However, transition metals, especially the Pt group metals, are often costly and toxic. Recently it has been shown that the asymmetric reduction of imines using enantioenriched N-heterocyclic phosphines, or NHPs, is feasible, affording enantioenriched secondary amines. One limiting factor is the ability to tune the catalyst due to the scarcity of commercially available starting materials, namely enantioenriched primary amines. The purpose of this project is to synthesize chiral amines to generate sterically constrained NHPs in order to improve the stereoselectivity in imine hydroboration reactions. This work reports the successful synthesis of sterically constrained ketones from commercially available aldehydes; as well as the transformation of said ketones into chiral but racemic amines. The racemic amines will be resolved via enzymatic or kinetic resolutions, then converted into the corresponding NHPs for use in the asymmetric hydroboration of imines.

Synthesis of Iron Complexes Supported by Mixed Donor P, N Ligands: Applications Towards Catalytic Amide Reduction

Dylan Hale and Laura Turculet

Dalhousie University

Division: Undergraduate Inorganic

Catalysts that utilize first row transition metals such as iron have recently attracted significant attention due to the relatively high abundance and low cost of the first row metals. While such sustainable catalysts are being utilized for a variety of applications, research in the Turculet group has targeted the catalytic hydrosilylation of carbonyl substrates using first row transition metal amido complexes as precatalysts. Whereas the hydrosilylation of aldehydes, ketones and, to a lesser extent, esters is well established in this regard, relatively few reports on the hydrosilylation of amide substrates appear in the literature. Towards this end, the study presented herein details an investigation into the use of iron precatalysts for the hydrosilylation of tertiary amides to amines.

This presentation focuses on the development of a family of multidentate, mixed donor, monoanionic P,N ligands and the utility of their corresponding (P,N)Fe(II) complexes as precatalysts in the hydrosilylation of tertiary amides. Efforts to optimize this reactivity via ligand design are presented. Results obtained thus far suggest that reducing the steric bulk associated with the N-donor leads to the formation of $Fe(P,N)_2$ species, where two ligand equivalents coordinate to the metal center. Additional results indicate that the addition of a second L-type donor to the ligand framework lends the complex too much stability, decreasing its reactivity. Attempts to prepare a P,N bidentate ligand variant with reduced steric bulk at the P-donor are also described.

One-Pot Crosslinking System for CO2-Switchable Coatings

Caroline Spence-Elder, Jaddie Ho, Bhanu Mudraboyina, Rui Resendes, and Philip Jessop

Queen's University

Division: Undergraduate Organic

Solvent coating formulations (e.g. organic paints) outperform aqueous coating formulations (e.g. latex paints) but emit volatile organic compounds, which are hazardous to the environment and health. Therefore, a replacement coating formulation is desired. A CO_2 responsive polymer in an aqueous solution was developed. A hydrophobic amine polymer can become a hydrophilic polymer by amine protonation in the presence of CO_2 and water. However, the CO_2 responsive coating remained out-performed by the solvent coating formulations. A one-pot crosslinking system to increase solvent resistance was developed through the use of diepoxides and CO_2 responsive polymers. The crosslinking reaction is controlled through amine protonation. In the carbonated aqueous solution (pre-film process) the protonated polymer is unable to react with the crosslinker. The evaporation of CO_2 (e.g. through the drying process) deprotonates the polymer allowing it to freely undergo the crosslinking reaction, resulting in a clear continuous solvent resistant coating.

Advances in Ancillary Ligand Design for Enabling Nickel Catalyzed C-N Cross-coupling

Chris Lavoie, Mark Stradiotto, and Erin Johnson

Dalhousie University

Division: Graduate Inorganic

The palladium catalyzed C_{sp2}-N cross-coupling of NH substrates and aryl (pseudo)halides (i.e., Buchwald-Hartwig Amination, BHA), is employed broadly in synthetic organic chemistry for the synthesis of aryl amines and related derivatives. Notwithstanding the broad impact of BHA in basic and applied research, the increasing difficulty for end users to procure precious Pd on larger scales has led to intensified interest into the development of coupling methodologies that utilize inexpensive, non-precious metals. In this regard, nickel has proven to be highly versatile in catalyzing the C_{sp2}-N coupling of a broad spectrum of synthetically attractive reagents (e.g., ammonia, alkyl amines, anilines, azoles, amides, etc.).[1-2] Despite such advances, our understanding of the influence of ancillary ligand ligation on catalyst performance is currently lacking, which severely impedes the development of superlative Ni catalysts that rival state-of-the-art catalysts from the BHA domain. This inspired a combined experimental and computational investigation[3] into the influence of ancillary ligand structure on key elementary steps in conventional C_{sp2}-N coupling, which has guided the design of superlative ligand classes based on bisphosphines. The findings of this investigation will be the focus of this presentation, and should provide a useful platform for further ancillary ligand design studies in the context of homogenous nickel catalysis.

1. C. M. Lavoie, P. MacQueen, M. Stradiotto and co-workers: *Nature Comm.* **2016**, 7, 11073; *Chem. Eur. J.* **2016**, *22*, 18752.

2. C. M. Lavoie, R. McDonald, E. R. Johnson, M. Stradiotto, *Adv. Synth. & Catal.* **2017**, *359*, 2972-2980.

Muon Spectroscopy Investigation into Hyperfine Structure, Reactivity, and Intrinsic Properties of Gold Nanoparticles Stabilized by Berry Extract

Andrew Linton and Dr. Khashayar Ghandi

Mount Allison University

Division: Undergraduate Materials

Muon spin resonance (μSR) spectroscopy is increasingly recognized as a useful and versatile tool for exploring hyperfine structure, reactivity, and intrinsic magnetic properties of metal nanoparticles. A green chemistry technique, μSR allows solid samples to be analyzed directly, facilitating minimal sample preparation and use of toxic solvents. This investigation explores μSR characterization of novel gold nanoparticles (AuNPs) stabilized by aqueous extract of *Sorbus decora* berries. Transverse field, longitudinal field, and zero field μSR experiments, carried out at the Japan Particle Accelerator Research (J-PARC) facility, reveal a wide range of characteristic chemical and physical information. Specifically, trends in muon asymmetry and relaxation provide insight into temperature and field dependence of surface radical reactions and magnetic dynamics of the AuNPs. Complemented by magnetic susceptibility testing, the μSR results support that the prepared AuNPs exhibit antiferromagnetism, a magnetic state which has not been previously reported for gold. Practical applications of antiferromagnetism, largely overlooked in recent years, show promising potential in spintronics and superconductivity.

Purification and Total Acid Number Reduction of Raw Diesel Via Column Chromatography

Ernlie Publicover and Kai E. O. Ylijoki

Saint Mary's University

Division: Undergraduate Organic

Crude petroleum products have impurities that are harmful to industrial equipment, vehicles, and the environment. The American Society of Testing and Materials (ASTM) is a regulatory body that controls the standards for different classes of fuel. These regulations can include acidity, sulfur content, flash point, and many more parameters. ASTM has different standards depending on the type of fuel. In this research, the standards for road going diesel (ASTM D975) will be used. An unrefined diesel product provided by an industrial collaborator will be upgraded to reach the ASTM standards for acidity and sulfur content. Also, the industrial collaborator asked us to improve the colour and smell of the diesel. Acidity is measured by the total acid number (TAN) with the units of mg of KOH per g of diesel. The TAN value was lowered through acid-base neutralization using different conditions. A novel technique of using column chromatography was developed to purify the diesel. This technique greatly improved the colour and smell, with colour ranging from an initial brown colour to green or colourless. The odour could be converted to a petroleum like odour from a strong initial camp fire burning aroma. The column was optimized to be run without solvent and the stationary phase recycled. The column can purify up to 800 mL of diesel per 100 g of silica gel and has a recovery of 70%. The TAN value was also reduced to less than 0.03 mg of KOH per gram of diesel using this method of purification.

What's POPin'? A Synthesis of Dithiol-Linked Porous-Organic Polymers

Laurie J. Donnelly and Dr. Michael J. Katz

Memorial University of Newfoundland

Division: Undergraduate Materials

Porous-Organic Polymers (POPs) have been of interest recently due to the high surface area per weight of porous materials and the processability of polymers;[1] along with their relative stability in comparison to other 3D polymers such as metal organic frameworks (MOFs). Due to their high surface area per mass and relative stability, POPs are useful for applications in catalysis[2], gas storage[2] and separations[3], and optoelectronic devices.[4] A common problem in POP synthesis however, is that they are formed from cross-coupling reactions that often require metal catalysts and/or high heats, which can limit the functionality of the polymer. If a metal-free and room temperature synthesis could be determined, then a new class of materials could be readily made and examined. For this purpose, a POP assembled through the reaction between a thiol and alkyne was targeted as alkynes and thiols readily undergo an addition reaction under UV light.[5] A two component system, as selected, allows for modifications pre-assembly that may not be possible in a single component polymer, thereby increasing the number of functional groups that could be incorporated into the POP (figure 1). This presentation will focus on the progress towards the synthesis of various thiol-containing porous-organic polymers. The high surface area and relative stability of such a thiol-containing polymer could allow for applications in the removal of heavy metals from water.

1. Tan, L.; Tan, B.Chem. *Soc. Rev.* **2017**, 46, 3322–3356.

2. Kaur, P.; Hupp, J. T.; Nguyen, S. T. *ACS Catal.* **2011**, 1, 819–835.

3. Zhang, X.-M.; Ding, X.; Hu, A.; Han, B.-H. *Polymer***2017**,118, 249 – 255.

4. Bildirir, H.; Gregoriou, V. G.; Avgeropoulos, A.; Scherf, U.; Chochos, C. L. *Mater. Horiz.* **2017**, 4, 546–556.

5. Lowe, A. B. *Polymer* **2014**, 55, 5517 – 5549.

Diversion of Crab Bodies from Landfill – Generation of High Value Biochar

Haley Armstrong and Stephanie MacQuarrie

Cape Breton University

Division: Undergraduate Organic

Every year Louisbourg Seafoods Ltd. sends approximately 1000 tons of crab waste to landfills. Transport of this waste material is not only costly for them, but it is also burning a significant amount of fossil fuels. Louisbourg Seafoods Ltd. is currently investing in efforts to identify an environmentally beneficial disposal method for the considerable amount waste generated by processing of snow crab. For every crab processed one third of each crab body will end up in Canadian landfills. A proposed method for this waste stream is to generate biochar. Crab based biochar was generated by slow pyrolysis at 400°C for 4 hours. The generated biochar was fully characterized by FT-IR, BET, XRD, TEM, and GC-MS. The crab biochar was found to have a surface area of 16.3 m^2/g by BET analysis. FT-IR and XRD showed there was a significant amount of calcium carbonate in the crab biochar. XRD showed the crystal structure is calcite. A Palladium-Zinc-CaCO3 catalyst was generated to catalyze the hydrogenation of alkynes to alkenes. This catalyst is hypothesized to be stereospecific for the cis-alkene product. The performance of the catalyst was analyzed by a simple hydrogenation of 2-butyne-1,4-diol. The Pd-Zn-CaCO3 catalyst was active, however the product produced was butane-1,4-diol instead of cis-2-butene-1,4-diol. This shows the catalyst is not stereospecific in its current state.

Low Surface Area Alloy/GIC Composites for Lithium Ion Battery Anodes

Shayne Gracious and Mark Obrovac

Dalhousie University

Division: Undergraduate Materials

Composite materials for lithium ion battery anodes were synthesized by combining various powders with poly(acrylic) acid (PAA). These powders were based on combinations of a Si-Fe alloy and an aluminosilicate glass. It was found that the composite materials showed an increase of particle size relative to that of the initial Si-Fe alloy while retaining the Si-Fe crystalline phases. Furthermore, the introduction of aluminosilicate glass improved the water stability of the composite materials. The use of high shear mixing as a method of electrode slurry formation was also explored. This yielded electrodes that had reduced polarization, but formed crystalline $Li_{15}Si_4$ phase throughout cycling. The use of the composite materials in these electrodes suppressed the formation of this phase. Despite the formation of this phase in some of these electrodes, they showed good cell performance.

Bis(diarylethynyl-methylene)dihydroantracenes: Synthesis, properties and tunable aggregation-induced emission

Matthew A. Johnson, Yuming Zhao, and Zahra Tabasi

Memorial University of Newfoundland

Division: Undergraduate Organic

Aggregation-induced emission (AIE) is a phenomenon in which a class of molecules do not exhibit solution phase emissions but become highly emissive in the solid-state or upon forming aggregates. A newly developed series of molecules, namely, bis(diphenylmethylene)dihydroacenes[1] have been found to exhibit this AIE effect through restriction of intramolecular rotation (RIR) around the phenyl bond, and restriction of intramolecular vibration (RIV) through the acene core. Herein, we examine the effect of extending such structures by an ethynyl unit, ideally they would exhibit a similar crystal packing and therefore undergo a comparable AIE mechanism. However, the extension of the phenyl unit causes lack of steric interactions which makes the RIR mechanism less likely and as a result we obtain differing results. In addition, it would appear that substitution controls the ability of the molecule to exhibit an AIE effect. Finally, attempts to cyclize one of the species to the corresponding tetra-substituted coronene will also be discussed.

1. Tang, Z. B. et al. *Chem. Sci.*, **2015**, *6*, 3538 – 3543.

Nanocomposites as Catalysts for Biomass Transformation in High Value Added Products

Andrew C. Duffy, Geniece L. Hallett-Tapley, and José Carlos Netto-Ferreira

St. Francis Xavier University

Division: Undergraduate Organic

The development of green processes to transform cellulose and lignin, the most abundant renewable biomaterials on Earth, is of the utmost importance for sustainability given their biocompatibility and potential as alternative fuels. Heterogeneous semiconductor photocatalysis is also central to this process. The structure, size and porosity of the solids can be manipulated to greatly improve catalytic activity. Moreover, visible light, ideally sunlight, can be exploited as a green energy source and converted into chemical energy in an environmentally benign manner. This contribution will discuss the design of multifunctional nanoparticle/Nb_2O_5 composites, exploiting the acidic, photocatalytic and photothermal capabilities of these heterogeneous materials to compliment the molecular characteristics of biomass. In particular, the photocatalytic aspect of these materials affords an opportunity to perform both oxidative and reductive processes after adsorption of one photon of light – increasing the effectiveness of these light-activated systems. Biomass conversion catalysts must be stable under hydrothermal conditions, *i.e.*, moderate temperatures and high water concentration, unfavourable in petroleum processing. The dual acidic/photocatalytic activities of niobium oxide materials may afford the ability to catalyze different reactions using the same catalytic bed in an effort to reduce the complexity of biomass transformations. Nanoparticles (Au and Ag) will be used to extend the response of the material into the visible region of the electromagnetic spectrum, due to their unique absorption characteristics. The catalytic capacity of several nanocomposites will be discussed, as well as the potential reusability of these materials, given the focus on renewable resources and sustainable green chemistry initiatives.

Structures of Glutathione Complexes with Alkali Metals by IRMPD Spectroscopy and Computational Methods

Kelsey Menard, Travis Fridgen, and Sharifi Mahsa

Memorial University of Newfoundland

Division: Undergraduate Physical, Theoretical, and Computational

The structures of alkali metal complexes of glutathione were studied by infrared multiple photon dissociation (IRMPD) spectroscopy and computational methods. The ions were produced by electrospray ionization (ESI) and isolated in the gas phase in a Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer in the 2700-4000 cm^{-1} region, and isolated in a modified Paul-ion trap mass spectrometer in the 900-1900 cm^{-1} region. The experimental IRMPD spectra in the higher energy region displayed bands corresponding to O-H stretching in all cases, and N-H stretching in the case of K, Rb, and Cs. The experimental IRMPD spectra in the lower energy region displayed bands corresponding to C=O stretching, CH_2 and CH_3 bending, C-N-H bending, C-O-H bending, and C-O stretching. Structures were optimized and IR spectra were computed at the B3LYP/6-31+G(d,p) level of theory on all atoms except Rb and Cs, to which the Def2SVP basis set and effective core potentials were applied. The computed IR spectra for the lowest energy structures were in excellent agreement with the experimental IRMPD spectra in the fingerprint region and were in relatively good agreement in the C-H/N-H/O-H stretching region. The structures and relative energies of glutathione alkali metal complexes were studied by Liu et al using DFT methods.[1] In their investigation, the lowest energy structures involved metal cations pentacoordinated to four oxygen atoms and one nitrogen atom. However, in our investigation, the lowest structures determined involved complexation of the metal ions to the carbonyl group and the carboxyl group of glutamic acid, and to the carboxyl group of glycine.

1. Liu, H.; Xia, X.; Li, Y.; Wang, H.; Li, Z. Theoretical study on the interaction of glutathione with group IA (Li^+, Na^+, K^+), IIA (Be^{2+}, Mg^{2+}, Ca^{2+}), and IIIA (Al^{3+}) metal cations. *Struct. Chem.* **2013**, *24*, 251-261.

Targeted Soil Inoculation: Impact and Future Directions

Kaitlyn Blatt-Janmaat, and Clarissa Sit

Saint Mary's University

Division: Undergraduate Biological and Medicinal

Food security is an issue worldwide. To provide enough food for our growing population, new agricultural practices must be investigated to ensure the long term viability and sustainability of the industry. In an attempt to increase the growth and yield of agricultural crops, several practices utilized by early farmers are being re-examined and improved. Two of these methods include biochar addition and soil inoculation. Biochar is a porous, pyrogenic material with a high carbon content formed from the slow pyrolysis of carbon heavy biomass. Introduction into the soil has yielded improvements in vegetative growth and nutrient retention. Soil inoculation is the practice of introducing beneficial microorganisms into the soil of the target host plant. When performed correctly, improvements in vegetative growth and plant immune response have been observed. A biochar-microbe composite has been produced and utilized as a means of targeted soil inoculation. Variable impacts on the vegetative growth, volatile production, and nitrogen content of plants has been observed with this technique. Implications for potential plant products, particularly wine, and future areas of research will be discussed.

Cyclometalated Ru(II) Dyads as Highly Selective Photosensitizers in Photodynamic Therapy

Anderson M. Fuller[1], Sherri A. McFarland[1], Colin G. Cameron[2], Goutam Ghosh[1], Tariq Sainuddin[1], Julia A. McCain[1], Susan M.A. Monro[1], Huimin Yin[1], and Marc W. Hetu[2]

[1]Acadia University
[2]The University of North Carolina at Greensboro, Greensboro, NC, USA

Division: Undergraduate Physical, Theoretical, and Computational

Photodynamic therapy (PDT) is a form of cancer treatment that utilizes nontoxic, light-responsive compounds that can be activated with photons to destroy cancer cells with spatiotemporal selectivity. Historically, porphyrin-based compounds have been used as photosensitizers and function by producing cytotoxic singlet oxygen ($^1O_2$) from triplet □□* excited states. We have invested efforts into developing coordination complexes as alternatives to these organic systems to access additional excited states that employ oxygen-independent mechanisms for photocytotoxicity. In this study, we developed Ru polypridyl complexes of the type $[Ru(dmb)_2(LL)]^+$ that incorporate C^N ligands with differing number of rings in the of □-oligothienyl functional ligand. These Ru(II) C^N complexes are both more photochemically stable and have red-shifted absorption profiles. These are attractive properties that triggered an investigation into the less studied domain of C^N complexes over their more popular counterpart, Ru(II) N^N complexes. The investigation on these four complexes demonstrated that as we increase the length of the □-expansive functional ligand, we getincreased access to ^{3}IL states, an increased phototherapeutic index (PI) and we found that this group of metal complexes could serve as highly selective chemotherapeutic agents and others are extremely potent photocytotoxic agents.

Investigation of the DNA binding domain on nickel-responsive regulator *Helicobacter pylori*'s NikR using cysteine mutants

Tam Pham, Deborah Zamble, Karina Baksh, and Jeremy Wong

University of Toronto

Division: Undergraduate Biological and Medicinal

The study's primary goal is to understand the structural changes of transcriptional regulator NikR in *Helicobacter pylori* (*H.pylori*). Using the ^{19}F-BTFMA chemical tag attached to cysteine residues, we aim to use ^{19}F-NMR to examine structural changes in *H.pylori* NikR (HpNikR) at different labelled regions. The mutant T3C, which located on the DNA binding domain, was subjected to this chemical ^{19}F-tag method. T3C-HpNikR demonstrated similar secondary structure as wildtype. It also showed a higher nickel loading ratio and lower DNA binding affinity than wildtype with the chance of oligomer formation at high concentrations. The labelled ^{19}F-T3C mutant appeared to lose its oligomerization. Preliminary data of the ^{19}F-T3C in the ^{19}F-NMR experiment showed certain correspondence to the cysteine residues; however, peak assignments were not finalized as further supporting data would be obtained in the future.

Conformation Dynamics of Keap1 Reactive Site Cys151 Changes due to Electrophilic Influences

Archita Adluri and Dr. C Rowley

Memorial University of Newfoundland

Division: Undergraduate Physical, Theoretical, and Computational

Chronic and acute inflammation is often attributed to oxidative/electrophilic stress in cells. Although many mechanisms and pathways exist to deal with this issue, one main pathway involving the regulation of the Keap1-NRF2 system is not fully understood1. On the path to creating targeted drugs towards oxidative/electrophilic stress, the sensing mechanisms must be understood. In this study, we created a computational model of the Keap1 homodimer starting from a crystal structure of a keap1 mutant2 (PDB 4CXI). The point mutations used to obtain a diffraction-quality crystal were corrected computationally. From this model, the local environment of a therapeutically important cysteine residue3 (Cys151) was analyzed. Two histidine's on the surface of this Cys151 local environment - His1289 and His154 - were examined for their potential protonation state in solution. The His129 was shown to switch conformations and move its imidazole ring ~5Å compared to crystal structure data, indicating it is potentially not the native conformation. We did not observe any conformational changes in the His154 when protonated along with His129 indicating this may be present in the protein native state.

Further studies are needed to investigate the protein on a lager scale as well as the effect of various electrophilic moieties binding to the cysteine thiol and their effect on the structure.

1. Nguyen, T.; Nioi, P.; Pickett, C. B. The Nrf2-Antioxidant Response Element Signaling Pathway and Its Activation by Oxidative Stress. *J. Biol. Chem.* **2009**, *284* (20), 13291–13295 DOI: 10.1074/jbc.R900010200.

2. Cleasby, A.; et al. Structure of the BTB Domain of Keap1 and Its Interaction with the Triterpenoid Antagonist CDDO. *PLoS One***2014**, *9* (6), 15–21 DOI: 10.1371/journal.pone.0098896.

3. Rachakonda, G.; et al. Covalent Modification at Cys151 Dissociates the Electrophile Sensor Keap1 from the Ubiquitin Ligase CUL3. *Chem. Res. Toxicol.* **2008**, *21* (3), 705–710 DOI: 10.1021/tx700302s.

Utilizing micro-ecological activity against bat pathogen *Pseudogymnoascus destructans* as a means of discovering novel antimicrobial compounds

Jennifer Kolwich, Lindsay Donovan, and Clarissa Sit

Saint Mary's University

Division: Undergraduate Biological and Medicinal

White-nose syndrome (WNS) is an emergent disease in North American bat populations. Since the first documented case in New York just over a decade ago, WNS has spread to 32 states and 7 provinces, leading to population decreases of 90-100% in some sites.[1,2] The causative agent of WNS was determined to be the fungal pathogen *Pseudogymnoascus destructans* (*Pd*).[2,3] Recent studies that have had success at treating WNS utilize the status of *Pd* as an invasive species in the skin microbiome of North American bats; they have found that micro-ecological defenses of pre-existing cutaneous specimens could be the key in reducing the effect of the fungus. With this in mind, we have isolated and purified samples of cutaneous microbes from a colony of big brown bats. These purified strains have undergone pairwise assays against a closely related *Pseudogymnoascus* species, as well as Gram-positive and Gram-negative bacteria, to test for inhibitory activity. The metabolites of biologically active strains will be extracted, purified, and tested directly for antimicrobial activity. Fractions shown to have potent biological activity will be analyzed by mass spectrometry and unreported natural products will be characterized.

1. U.S. Fish & Wildlife Service, **2018**.

2. Blehert DS, et al. Science, **2009**, *323*, 227.

3. Lorch JM, et al. Nature, **2017**, *480*, 376–378.

Pyridine Hydroboration with a Diazaphospholene Precatalyst

Toren Hynes, Alex Speed, Erin N. Welsh, Robert McDonald, and Michael J. Ferguson

Dalhousie University

Division: Undergraduate Organic

This talk will describe the discovery and development of a pyridine hydroboration reaction catalyzed by a diazaphospholene hydride precatalyst. Pyridines bearing electron-withdrawing groups in the 3-position are hydroborated efficiently. This system features low catalyst loadings, fast reaction times at ambient temperature, and tolerance of other reducible functionality. A mechanism based on NMR studies is suggested.

Title: Ionic Core Dependence of Ionophilic Thiourea Organocatalysis in Ionic Liquids

Katherine Parsons and Robert D. Singer

Saint Mary's University

Division: Undergraduate Organic

The Morita-Baylis-Hillman reaction forms a carbon-carbon bond between an electron-deficient alkene and an aldehyde in an atom economic, albeit slow, reaction in the presence of catalytic tertiary amine or phosphine. Utilizing the methylpiperidinium derived ionic thiourea co-catalyst, **1**, in the Morita-Baylis-Hillman reaction between benzaldehyde and 2-cyclohexene-1-one with DABCO resulted in a rate acceleration and appreciable conversion to the product. Additionally, recycling of the methylpiperidinium thiourea organocatalyst, **1**, was attempted by entrainment in two ionic liquids. Comparison to other ionic thiourea organocatalysts used in this system will also be discussed.

Investigating Moderately Electron Donating Ancillary Ligands in Nickel-Catalyzed C(sp2)-N Cross-Coupling

Ryan McGuire, Mark Stradiotto, and Jillian S. Clarke

Dalhousie University

Division: Undergraduate Inorganic

The optimization of Pd-catalyzed C(*sp*^{2})-N cross-coupling (i.e. Buchwald-Hartwig Amination, BHA) has led to the development of several highly effective ancillary ligands.[1] Indeed, for both benchtop and industrial-scale applications, BHA is a desirable protocol for the synthesis of bio-active (hetero)aniline derivatives.[2] Despite the utility of BHA, the price and scarcity of Pd inspires the implementation of more Earth-abundant base metals to affect similar transformations. The Stradiotto group has recently initiated a research program focused on the application of Ni-catalysis for the formation of C(*sp*^{2})-N bonds.[3]Notably, given the divergent chemical properties of Pd and Ni,[4] ancillary ligands that are successful in BHA are not always effective when re-purposed for use in Ni-catalyzed amination,[5] thereby creating motivation for the design of new and effective ligands for such reactions. The Stradiotto group has recently developed PAd-DalPhos, a bisphosphine ligand designed for Ni-catalyzed C(*sp*^{2})-N cross-coupling, which has addressed several difficult catalytic transformations including the mono-arylation of both primary amines and ammonia.[3] The success of sterically encumbering yet moderately electron donating PAd-DalPhos implies that ancillary ligands that meet these criteria may indeed be advantageous in Ni-catalyzed amination chemistry. In this presentation, our progress in developing sterically encumbering and moderately electron donating ancillary bidentate ligands for use in Ni-catalyzed C(*sp*^{2})-N cross-coupling will be described.

1. (a) Surry, D. S.; Buchwald, S. L. *Angew. Chem. Int.Ed.* **2008**, 47, 6338-6361;
   (b) Louie, J.; Hartwig, J. F. *Tetrahedron Lett.* **1995**, 36, 3609-3612.

2. Ruiz-Castillo, P.; Buchwald, S. L. *Chem. Rev.* **2016**, 116, 12564-12649.

3. Stradiotto, M. and co-workers *Nat. Commun.* **2016**, 7, 11073.

4. Stradiotto, M. and co-workers *Adv. Synth. Cat.* **2017**, 359, 2972-2980.

5. Han, F.-S. *Chem. Soc. Rev.* **2013**, 42, 5270-5298.

Synthesis of water soluble curcumin analogs

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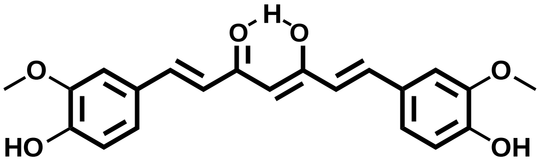
Division: Undergraduate Organic

Curcumin is the active ingredient in turmeric, a heavily consumed spice in South-east Asia. Curcumin possesses significant health benefits including cancer chemopreventative properties. However, it has poor bioavailability. To address this predicament, cyclic amine containing analogs of curcumin are being synthesized while retaining the diarylheptanoid framework of curcumin. The results obtained thus far will be presented.



Curcumin

Progress toward an asymmetric synthesis of pallescensin-1 and derivatives

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Division: Undergraduate Organic

Furanosesquiterpenoids are a class of structurally diverse natural products containing15 carbons in total and at least one furan. Pallescensins are a family of furanosesquiterpeneoids first isolated in 1975 from the marine sponge *Disidea pallescens*.[1-3]The pallescensin family consists of 10 compounds: three monocyclic compounds with an additional 3-substituted furan named pallescensin-1, -2, and -3, and seven compounds named pallescensins A-G featuring a bicyclic ring system plus a 2,3-disubstituted furan. This work focuses on an expedient synthesis of pallescensin-1 (**1**). The strategy is centered around a C5-7 bond disconnection which was envisioned to be the most fruitful in terms of devising an asymmetric route toward this molecule. The molecule can thereby be broken down into two coupling partners, a bromofuran (**2**) and an enone (**3**), whose synthesis has been completed and will be described. Development of the key copper-mediated conjugate addition of these two coupling partners is underway. Synthetically, we next envision a unified approach to the whole pallescensin family utilizing our key coupling along with more modern selective oxidative cyclization chemistry from our advanced intermediates. The synthetic work described includes synthesis of key intermediates and efforts toward synthesis of the final target via the copper-mediated conjugate addition.

1. Cimino, G.; De Stefano, S.; Guerriero, A.; Minale, L. *Tetrahedron Letters*, **1975**, 17, 1417-1420.
2. Cimino, G.; De Stefano, S.; Guerriero, A.; Minale, L. *Tetrahedron Letters*, **1975**, 17, 1421-1424.
3. Cimino, G.; De Stefano, S.; Guerriero, A.; Minale, L. *Tetrahedron Letters*, **1975**, 17, 1425-1428.

Bismuth Complexes of an Ambidentate Phosphorus-Amine Ligand

Robert D. Riley[1], Jason A. C. Clyburne[1], Diane A. Dickie[2], Michael A. Land[1], Richard A. Kemp[2], Charles L. B. Macdonald[3], and Katherine N. Robertson[1]

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[3] University of Windsor, Windsor, Ontario

Division: Undergraduate Inorganic

Bismuth is the heaviest metal of the p-block elements and it has found diverse applications in catalysis, medicine, and materials chemistry. Surprisingly, there are no reports of bismuth chemistry with the most common ambidentate pincer ligand (bis(diisopropylphosphino)amine). We have explored this chemistry and isolated a number of coordination complexes exhibiting Bismuth – Phosphorus bonds. Experimental results will be discussed and theoretical studies will be reported in this oral presentation.

Electrochemical-Surface Enhanced Raman Spectroscopy (EC-SERS) for Bacterial Screening

Taylor Lynk, Clarissa Sit, and Christa Brosseau

Saint Mary's University

Division: Undergraduate Analytical

The lack of efficiency of current methods for bacterial screening has prompted an increasing interest in developing a cost-effective, rapid, and sensitive alternative for applications in all sectors of society. This project aims to explore a new detection platform for bacterial screening by coupling an applied electric potential with surface-enhanced Raman spectroscopy (SERS); a technique termed electrochemical surface-enhanced Raman spectroscopy (EC-SERS). The goal of using this technique is to improve upon the sensitivity and reproducibility of normal SERS to allow for rapid, point-of-need bacterial detection and identification. This project first shows the EC-SERS characterization of the commonly observed nucleotide breakdown products that dominate the SERS spectra of bacteria: adenine, guanine, xanthine, hypoxanthine, uric acid, 5'-adenosine monophosphate (AMP), and guanosine. This work then concentrates on developing a sample preparation method to be used to study bacteria using EC-SERS for the first time. The results of this project demonstrate the improvement of the SERS spectra for both E. coli K-12 and B. megaterium bacteria when an electric potential is employed, highlighting the great promise of EC-SERS for use as a fast and affordable bacterial screening method. EC-SERS is also shown to be able to discriminate between the two strains of bacteria by employing a spectral database containing the EC-SERS data for the nucleotide breakdown products.

Combining calculation with experiment to study interphase formation reactions in lithium-ion cells

David Hall and Jeff R. Dahn

Dalhousie University

Division: Graduate Physical, Theoretical, and Computational

To further progress the adoption of electric vehicles and other high power energy storage applications, it is desirable to develop lithium-ion cell chemistries that offer longer lifetimes at high temperatures and cell voltages, without significantly increasing the cost. The introduction of sacrificial electrolyte additives on the order of a few weight percent is a practical method to form protective solid-electrolyte interphase (SEI) layers that limit electrolyte decomposition during cell storage and operation. In recent years, significant efforts have provided new understanding of the underlying chemistry of several such additives.

This work will present how density functional theory (DFT) calculations have been used to explore the underlying chemical reactions leading to SEI formation. Two sulfur-containing additives, prop-1-ene-1,3-sultone (PES) and ethylene sulfate (DTD), will be discussed. The DFT results offer new insight into the onset potential and reaction products of electrochemical reduction. By pairing DFT with a diverse set of experimental techniques, including X-ray photoelectron spectroscopy, isothermal microcalorimetry, solid-state nuclear magnetic resonance spectroscopy, gas volume measurements, and electrochemical techniques, new SEI components are proposed for each additive.

In general, the results in this work confirm previous recommendations that a wide variety of experimental techniques, coupled with computational methods such as density functional theory, can offer new insights into the underlying chemistry of SEI formation in lithium-ion cells. It is hoped that future work can apply the results of this work to understand what makes a ‘good’ electrolyte additive and, ultimately, to design new and improved electrolyte cell chemistries.

An Exploration of 2D-LC-SERS: A Novel Detection Modality for Multidimensional Chromatography

Melanie Davidson and Dr. Christa Brosseau

Saint Mary's University

Division: Graduate Analytical

Multidimensional liquid chromatography (2D-LC) provides substantially better resolving and separating power than conventional high pressure liquid chromatography (HPLC), and over the past decade has been applied in many different fields of chemistry.[1] The current gold standard for detection modalities in conjunction with LC is mass spectrometry (MS). However, this technique is data heavy, it isn't portable, and the instrumentation can be very expensive.[2] This research will couple the emerging technique of 2D-LC with the sensing power of surface-enhanced Raman spectroscopy (SERS) as a new detection modality. In order to exploit this detection technique, a SERS substrate must be optimized. Many different 3D-substrates were investigated for their use in phenolic acid detection. It was found that generic laboratory filter paper covered in pyridine functionalized silver nanoparticles gave the most promising results. These substrates will be used for further investigation and coupling of SERS to 2D-LC.

1. Stoll, D. R.; Carr, P. W. *Anal. Chem.* **2017**, *89* (1), 519–531.

2. Mandal, S. M.; Chakraborty, D. In *Natural Products: Phytochemistry, Botany and Metabolism of Alkaloids, Phenolics and Terpenes*; Ramawat, K. G., Mérillon, J.-M., Eds.; Springer Berlin Heidelberg: Berlin, Heidelberg, 2013; pp 2047–2059.

Synthesis and Characterization of Edaravone Analogs: Novel Therapeutic Approaches for Amyotrophic Lateral Sclerosis

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Université de Moncton

Division: Graduate Biological and Medicinal

Amyotrophic lateral sclerosis (ALS) is a condition primarily characterized by the selective loss of upper and lower motor neurons. Motor neuron loss gives rise to muscle tissue malfunctions, including weakness, atrophy, and ultimately paralysis, with death typically due to respiratory failure within 2 to 5 years of symptoms onset. The therapeutic approaches currently offered to ALS patients are unfortunately limited. Edaravone (3-methyl-1-phenyl-2-pyrazolin-5-one) is a newly approved drug given to patients for ALS treatment. The beneficial biological activities of Edaravone are notably due to its antiradical and antioxidant activities. Nevertheless, a better characterization of the molecular impacts underlying the positive effects of this drug remains to be performed. In addition, even though Edaravone is approved for the treatment of ALS, its beneficial effects are rather limited (Abe, K. *et al*. 2017). In this study, a series of Edaravone's analogs were synthesized and their antiradical and antioxidant activities were evaluated. Two compounds fared significantly better than Edaravone in all assays. These lead compounds were further tested *in vitro* on NSC-34 cells, a model used in ALS work, and reveal interesting information on the compounds' impact on select cell metabolites. Overall, this study was conducted to better understand the Structure Activity Relationship of the designed Edaravone's analogs. Two promising compounds were identified and will be further evaluated in the ongoing development of therapeutic approaches for patients diagnosed with ALS.

1. Abe, K *et al.*, *The Lancet Neurology* **2017,** *16* (7), 505-512.

Optimization and validation of ^{226}Ra measurements by ICP-MS in sediments after a simple acidic mineralization

Ben Yaala Hamza, Olivier Clarisse, and Delphine Foucher

Université de Moncton

Division: Graduate Analytical

If radiometric techniques (e.g. alpha, gamma, liquid scintillation spectrometry or radon emanation spectrometry) are commonly used to determine radium (Ra) concentration at trace level in sediment, they are laborious and time consuming in both terms of sample preparation and Ra measurement. Inductively coupled plasma mass spectrometry (ICP-MS) is an alternative method for rapid and precise measurement of radionuclides with long half-lives, such as radium-226. However, complex matrices of mineralized sediment may affect ICP-MS performances in terms of precision and accuracy: spectral interference, matrix effect and instrumental drift should be therefore considered. Impact of spectral interferences (^{208}Pb^{18}O, ^{138}Ba^{88}Sr, ^{139}La^{87}Sr, ^{140}Ce^{86}Sr, ^{186}W^{40}Ar...) were tested at natural and relevant sedimentary concentration for the iCAP-Q ICP-MS (Thermofisher) in standard (STD) and Kinetic Energy Discrimination (KED) analytical modes. In STD mode, several interferences were observed for ^{226}Ra analysis but became negligible in KED mode except for lead: ^{226}Ra concentration is overestimated by 25% for a sediment with Ra at 1 pg g^{-1} and Pb at 20 µg g^{-1}. Secondly, 8 different internal standards were tested to properly correct any matrix effect and instrumental drift: spikes recoveries of low ^{226}Ra levels were measured for 5 natural sediments (fluvial, estuarine or marine) mineralized using HF, HNO_3 and HCl acids. Matrix effect and instrumental drift on iCAP-Q ICP-MS were efficiently corrected using ^{103}Rh, ^{115}In, ^{195}Pt or ^{209}Bi. Determination of ^{226}Ra concentration in mineralized sediment by ICP-MS is rapid, simple and accurate once performed in KED mode and lead concentration considered (requiring matrix blank matching if needed).

Development of Gold Plasmonic Nanoarrays for Efficient SERS Sensing of Environmental Contaminants

Najwan Albarghouthi and Dr. Christa Brosseau

Saint Mary's University

Division: Graduate Analytical

Public attention to the water contamination raises an urgent need to develop effective and reliable methods to detect the presence of any organic compound in water such as, atrazine. The current detection techniques for instance, liquid chromatography, mass spectroscopy, or colorimetric methods, which usually require sophisticated and time-consuming steps or sample preparation besides a well-trained operator. Herein, surface enhanced Raman is a powerful vibrational spectroscopy technique that allows for highly sensitive structural detection of compounds. Significant signal amplification is observed on roughened surface of metal nanostructure. However, developing a novel nanomaterial as cost effective, sensitive, and reproducible substrate for surface-enhanced Raman spectroscopy (SERS) applications remains a major challenge. Therefore, Gold nanorods (GNR) are a great candidate for SERS substrates, their importance rises from their LSPR excitation by light, which generates a strong signal due to their anisotropic shape. While great progress has been made in the synthesis of gold nanorods, relatively less success has been achieved towards ordering such structures into 2- and 3- dimensions in an effort to have a more uniform and robust sensing platform. This research work will explore two methods for the creation of multidimensional gold nanorod (GNR) arrays using both induced evaporation and Langmuir-Blodgettry.

Photocatalytic Applications of AuNP/Perovskite Hybrids in C-C Bond Formation

Bry W. Crabbe, Dr. Geniece Hallett-Tapley, Dr. Brian MacLean, and Oliver P. Kuehm

St. Francis Xavier University

Division: Graduate Materials

Heterogeneous catalysis has garnered considerable attention over the past decade as a means of implementing more sustainable chemical routes through the use of environmentally benign energy sources (light) and minimizing undesirable toxic chemical waste and byproducts. Perovskite potassium niobium oxides are an underdeveloped class of semiconductor materials, with properties similar to TiO_2, that allow for ease of removal from reaction solutions due to its larger particle size. Nanoparticle functionalization (Au, Pd) of the potassium niobium oxide surface will enable greater charge separation on light activated semiconductor surface, allowing for more effective exploitation of its photoredox states. In the following contribution, the light-driven reactivity of these solids will be examined for applications in the photocatalytic C-C homocoupling reactions of iodobenzene and phenylboronic acid, respectively. Preliminary results illustrate proficient and selective coupling of the substrate molecules to form the coupled biphenyl product. Surprisingly, the monometallic, AuNP-potassium niobium oxide composites produces high product yield in iodobenzene coupling while PdNP-potassium niobium oxide hybrids perform best in the correspondingphenylboronic acid reaction. The effects of metal nanoparticle loading, metal nanoparticle properties, light source, reaction time, reaction components and recyclability of photocatalyst will be examined and directly correlated to the efficiency of light induced carbon-carbon bond formation.

Benchtop Borenium Catalysis

Blake Huchenski and Dr. Alex Speed

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Division: Graduate Organic

Borenium catalysis has undergone a rapid development in recent years, providing highly active catalysts in hydrogenation and hydrosilylation chemistry. Small molecules such as DABCO and lutidine have been highlighted in recent publications to stabilize borenium ions[1,2]. This chemistry has been applied in catalytic reactions using common boranes as reagents. However, these catalysts are often highly moisture sensitive and require dry conditions for use. Catalysts are often prepared before use, as the reagents used for preparation of borenium cations are themselves often active catalytically. This work provides an account of a new moisture tolerant system which provides access to borenium chemistry on the benchtop in common solvents without the use of solvent drying or purification. This system can also be applied to hydrogenation and hydrosilylation chemistry with the aid of carbene borane complexes[3].

1. Eisenberger, P.; Bailey, A. M.; Crudden, C. M. J. Am. Chem. Soc. 2012, 134 (42), 17384-7.

2. Denmark, S. E.; Ueki, Y. Organometallics 2013, 32 (22), 6631-6634.

3. Huchenski, B. S. N.; Adams, M. R.; McDonald, R.; Ferguson, M. J.; Speed, A. W. H. Organometallics 2016, 35 (18), 3101-3104.

New Materials from Waste-Derived Fish Oil

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Memorial University of Newfoundland

Division: Graduate Materials

Waste by-products from fish processing plants includes heads, bones, and skin, and is ~50 wt.% of the landed fish.[1] Finding uses for this waste would increase sustainability in the fishing and aquaculture industries. Fish oils have the potential to be converted into commercially important products, including epoxides, cyclic carbonates, and polyurethanes, using environmentally benign and non-toxic reagents. Fatty acid (FA) epoxides can be made using acetic acid and H_2O_2 in the presence of a catalytic amount of acid.[2] In the current research, GC-MS, ^{1}H, and ^{13}C NMR spectroscopy were used to characterize epoxidized fish oil. Monounsaturated oils, methyl oleate and oleic acid, as test substrates, were epoxidized achieving yields of 79%, and 85%, respectively. Salmon oil was also epoxidized, giving 2.73 epoxy groups per triglyceride. The synthesized FA epoxides can be reacted with $CO_2$and a catalyst to form cyclic carbonates. The cyclic carbonates can then react with environmentally sustainable bio-sourced amines to form polyurethanes. The polymers produced, as they will be 100% bio-derived, may show an enhanced biodegradability over traditional petroleum based materials.

1. F. M. Kerton, Y. Liu, K. W. Omari and K. Hawboldt, *Green Chem.*, 2013, **15**, 860.

2. J. Langanke, L. Greiner and W. Leitner, *Green Chem.*, 2013, **15**, 1173.

Synthesis, Characterization, and X-Ray Crystal Structures of Carbodicarbene Precursors

Michael A. Land, Jason A. C. Clyburne, Robert Riley, and Katherine N. Robertson

Saint Mary's University

Division: Graduate Organic

A modular method has been developed and used to synthesize a series of 1,3-*bis*(dimethylamino)-1,3-*bis*(donor)propenium salts. All salts were prepared *via* the condensation of 1,3-dichloro-1,3-*bis*(dimethylamino)propenium chloride with amines, phosphines, phenols, or thiols. All of the resulting salts were characterized by IR, NMR, EA, and HRMS, and they have also been studied using X-ray crystallography. Investigations are currently underway to find a way to prepare carbodicarbene complexes from these compounds.

Removing layered double hydroxides from precursors of NCA, a Li-ion battery electrode material

Aaron Liu, Jeff Dahn, Ning Zhang, Jim Li, and Hongyang Li

Dalhousie University

Division: Graduate Materials

As lithium ion battery technology expands into more demanding applications such as electric vehicles, attention has shifted away from the conventional $LiCoO_2$positive electrode material. Instead, nickel-rich materials such as $LiNi_{1-x-y}Mn_xCo_yO_2$ (NMC) and $LiNi_{1-x-y}Co_xAl_yO_2$ (NCA) have become attractive due to their lower cost, increased lifetime and increased safety. Coprecipitation is a common method to synthesize mixed metal hydroxides ($M(OH)_2$: M = divalent transition metals) as the precursor materials to the lithiated metal oxides. While the syntheses of divalent NMC precursor materials are well understood, the introduction of a trivalent cation, such as Al^{3+}, complicates the synthesis and affects the products significantly.[1] In order to balance the charge, an extra anion needs to be incorporated into the layered structure, resulting in the formation of a new layered double hydroxide (LDH) phase. The LDH phase is analogous to α-$Ni(OH)_2$, which are well studied due to its range of applications.[2] It is known that α-$Ni(OH)_2$ can be converted into β-$Ni(OH)_2$, which has no intercalated molecules, by a process called chemical ageing.[2] This is generally performed in concentrated alkaline solutions, usually at higher temperatures. In this work, $[Ni_{0.80}Co_{0.15}]_{0.95-x}Al_{0.05+x}(OH)_2$ ($x = 0, 0.05$) precursor materials were prepared by the coprecipitation method. The precursor materials were then washed in a solution of NaOH, filtered and dried. Temperature, NaOH concentration, and stirring time were varied to study their impact on LDH removal. Unwashed and washed samples were characterized by XRD, ICP-OES, TGA-MS, SEM and photographs. Recommended recipes for the production of competitive NCA hydroxide precursors are reported.

1. Zhao, X.; Zhou, F.; Dahn, J. R. *J. Electrochem. Soc.* **2008**, *155*, A642–A647.

2. Hall, D. S.; Lockwood, D. J.; Bock, C.; MacDougall, B. R. *Proc. R. Soc. A* **2014**, *471*, 20140792(1-65).

A New Synthetic Route to 2-Formyl Pyrroles from Knorr-Type 2-Thionoester Pyrroles

Min Joon Kim, Dr. Alison Thompson, Sophie Gaube, and Michael Beh

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Division: Graduate Organic

In synthesizing multi-pyrrolic compounds such as dipyrrins, BODIPYs and prodigiosenes, the presence of 2-formyl pyrroles is essential because this functional group provides a carbon bridge by which to link to different pyrrole units. Therefore, it is critical to have a facile and high-yielding synthetic route to 2-formyl pyrroles. One of the most prominent methods of making 2-formyl pyrroles is to convert a 2-carboxylate (i.e. ester) pyrrole to a 2-H pyrrole followed by formylation.1,2 These reactions require harshly basic conditions as well as extraneous heating for an extended period of time. In this work, 2-thionoester pyrroles were studied. They were prepared via the thionation of esters using Lawesson's reagent.3Treating 2-thionoester pyrroles with Raney nickel, which is well known for its thiophilicity, resulted in successful reduction to give 2-formyl pyrroles. One drawback of synthesizing 2-thionoester pyrroles is that treatment with Lawesson's reagent is difficult to scale up. Therefore, a new Knorr-type synthetic route to 2-thionoester pyrroles was explored to avoid the use of Lawesson's reagent.

1. He, Y.; Lin, M.; Li, Z.; Liang, X.; Li, G.; Antilla, J. C. Org Lett. 2011, 13, 4490.

2. Shah, S.; Lee, C.; Jeong, B. S. Org. Biomol. Chem. 2016, 14, 4829.

3. Groves, B.; Smithen, D.; Cameron, S.; Thompson, A. RSC Adv. 2016, 6, 69691.

Alkene Isomerizaton-Hydroboration Catalyzed by First-Row Transition Metal (Mn, Fe, Co, and Ni) N-Phosphinoamidinate Complexes: Origin of Reactivity and Selectivity

Casper Macaulay, Mark Stradiotto, Laura Turculet, Samantha J. Gustafson, Steven M. Bischof, Orson L. Sydora, and Daniel H. Ess

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Division: Graduate Inorganic

Remote functionalization of alkene-containing substrates facilitated by metal-catalyzed alkene isomerization is an attractive method for the synthesis of value-added materials. We have developed a three-coordinate N-phosphinoamidinate (PN) Co complex that is capable of performing the isomerization-hydroboration of internal alkenes with HBPin whereby exclusive terminal selectivity is achieved[1]. In this presentation, we report on our efforts to extend this chemistry to isostructural PN 3d transition metal complexes. The notable differences in reactivity and selectivity that are observed are justified both computationally and experimentally through analysis of potential catalytic intermediates.

1. a) Ogawa, T.; Ruddy, A. J.; Sydora, O. L.; Stradiotto, M.; Turculet, L. Organometallics 2017, 36, 2, 417-423.

   b) Ruddy, A. J.; Sydora, O. L.; Small, B. L.; Stradiotto, M.; Turculet, L. Chem. Eur. J. 2014, 20, 43, 13918-13922.

Regioselectivity Studies of Anionic 5-exo/6-endo-*dig* Cyclization toward Pyrrolone and Pyridinone

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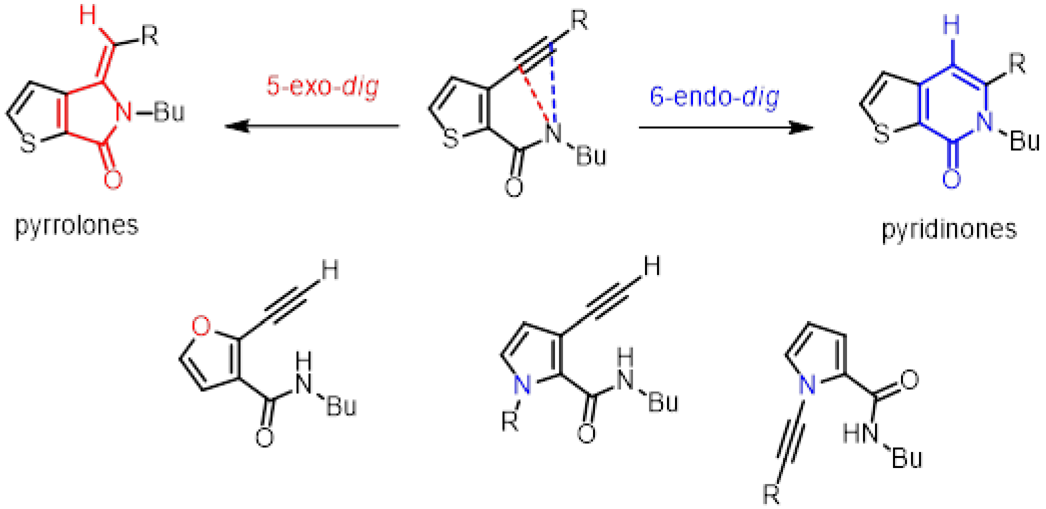
Division: Graduate Organic

Thieno-, furano-, and pyrrolo-alkynylamides were synthesized and cyclized into pyrrolone (5-exo-*dig*) and pyridinone (6-endo-*dig*) products. The competing cyclization pathways were explored experimentally and computationally, providing access to these new class of heterocyclic molecules currently unavailable by other methods.[1] The 5-exo-dig cyclization pathway is usually disfavoured in heterocyclic systems, and 6-endo products are often both the kinetic and thermodynamic products. Shifting the favourability toward the 5-exo-dig can be achieved by changing factors such as heteroatom identity and position in the heterocycle, and functional groups attached on the alkyne and N-pyrrole positions. A series of computational studies was performed to provide further insight into the 5-exo and 6-endo dig pathways in these heterocyclic systems. Theoretical predictions were found to reproduce experimental results, highlighting the predictive capabilities of the computations in determining preferred products.



1. Infante, G.; Eisler, S. *Can. J. Chem.*, **2017**, 95, 415-423

Coordination of Model Naphthenic Acids to Magnesium and Zinc

Matthew Laprade, Jason Clyburne, Bitu Hurisso, and Katherine Robertson

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Division: Graduate Inorganic

Naphthenic acids are naturally occurring carboxylic acids that have the general formula of $C_nH_{2n+z}O_2$. They are an undesirable component of bitumen which gives rise to a number of harmful effects. Naphthenic acids have relatively high polarities compared to other organic molecules allowing them to be soluble in aqueous systems and also causing the acids to act as surfactants. This property of naphthenic acids is the initial reason why oil spills are environmentally devastating. Industrially, naphthenic acids are detrimental as they cause corrosion to metal infrastructure.

Surprisingly few systematic studies have been done to understand their coordination with metal ions. Model naphthenic acids are shown to undergo coordination reactions with different metal ions important in aqueous chemistry. The metal center atoms, zinc and magnesium, were selected based on industrial oil pipeline use of sacrificial anodes and anti-corrosion additives. The metal ions are also present naturally within bitumen. The crystal structures of multiple compounds have been determined by X-ray crystallography. These structures include, but are not limited to, $Zn(C_7H_{12}O_2)_2(H_2O)_2$, $Mg(C_7H_{12}O_2)_2(H_2O)_4$, $Zn(C_8H_{14}O_2)_2(H_2O)_2$, and $Mg(C_8H_{14}O_2)_2(H_2O)_4$. All structures determined by X-ray crystallography have also been characterized by melting point, elemental analysis, infrared spectroscopy, and NMR spectroscopy.

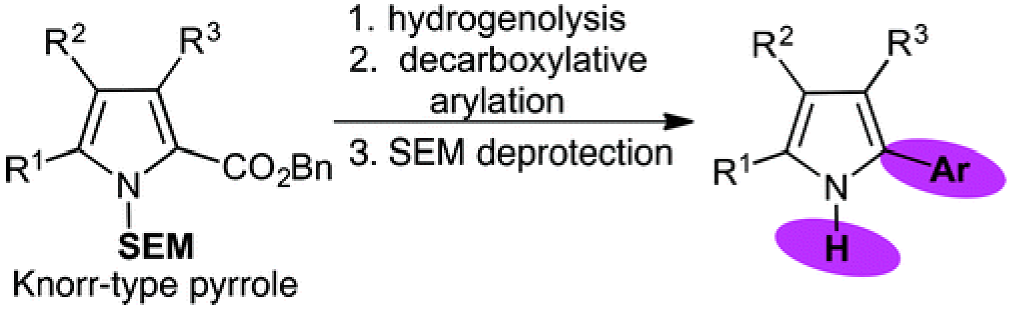
Decarboxylative arylation of substituted pyrroles N-protected with 2-(trimethylsilyl) ethoxymethyl (SEM)

Sarah M. Greening, Carlotta Figliola, Connor Lamont, Brandon Groves, and Alison Thompson

Dalhousie University

Division: Graduate Organic

Pyrroles are commonly used in the synthesis of pharmaceuticals, agrochemicals, dyes, perfumes and other organic compounds. Thus, significant effort has been made to develop methodology for the synthesis of pyrrolic derivatives. Transition-metal-catalyzed direct C-H arylation and decarboxylative arylation of pyrroles have been previously reported. However, the current literature reports the use of the fully unsubstituted pyrroles and do not illustrate the need to work with pyrroles bearing substitutions in the 3-, 4-, and 5- positions. Furthermore, current work involves pyrroles with N-alkyl and N-aryl protecting groups that prove challenging to remove and thus are impractical for use in synthetic development. This work reports the Pd-catalyzed decarboxylative arylation of pyrroles that are N-protected with 2-(trimethylsilyl)ethoxymethyl (SEM) and features substituents in the 3-, 4-, and 5-positions of the pyrrolic structure. Deprotection of the SEM group occurs under milder conditions comparative to current synthetic procedures involving decarboxylative arylation.



1. Figliola, C; Greening, S. M.; Lamont, C.; Groves, B. R.; Thompson, A. *Can. J. Chem.*, **2018**, 1-9.

Group 10 metal hydride complexes supported by new silyl pincer ligation: synthesis, characterization and catalytic activity

Luke Murphy and Laura Turculet

Dalhousie University

Division: Graduate Inorganic

Bis(phosphino)silyl (PSiP) pincer ligands developed in our group have been utilized in the preparation of numerous first, second and third-row late transition metal complexes that have demonstrated activity in a variety of challenging bond activation reactions (e.g. C-H, N-H, Si-C)[1] and catalytic processes.[2] Previous work involving square planar Group 10 metal complexes of the type (PSiP)MH (M = Ni, Pd, Pt; PSiP = κ^3-(2-Cy$_2$*P*C$_6$H$_4$)$_2$*Si*Me) has demonstrated the catalytic reduction of CO$_2$ to methane using tertiary silanes as the hydrogen source. Recently, we have developed a new class of PSiP ligand with strategic alterations in the ligand architecture. In this regard, this presentation will detail the synthesis of Group 10 metal hydride complexes supported by a novel PSiP ligand framework. Highly selective Ni-catalyzed CO$_2$ hydroboration to the formaldehyde level has also been achieved in this system, and a detailed study on solvent, temperature and ligand dependent interconversion between silyl hydrides and η^2-silanes has also been carried out.[3]

1. (a) Morgan, E.; MacLean, D.F.; McDonald, R.; Turculet, L.; *J. Am. Chem. Soc.* **2009**, *131*, 14234;
   (b) Mitton, S.J.; McDonald, R.; Turculet, L. *Angew. Chem. Int. Ed.* **2009**, *48*, 8568.

2. (a) Mitton, S.J.; Turculet, L. *Chem. Eur. J.* **2012**, *18*, 15258;
   (b) Takaya, J.; Kirai, N.; Iwasawa, N. *J. Am. Chem. Soc.* **2011**, *133*, 12980.

3. Murphy, L.J.; Hollenhorst, H.; McDonald, R.; Ferguson, M.; Lumsden, M.D.; Turculet, L. *Organometallics* **2017**, *36*, 3709.

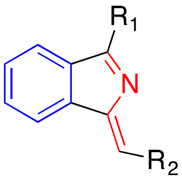
Synthesis and Electronic Properties of Benzo- and Thieno-pyrrole Derivatives

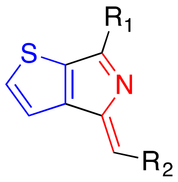
Brandon Christopher Fillmore and Sara Eisler

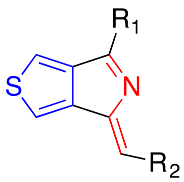
University of New Brunswick

Division: Graduate Organic

π-Conjugated organic molecules are of significant interest due to their ability to transmit electrical charge. In contrast to their inorganic counterparts, organic materials offer lower cost, higher flexibility, and easier tunability. Their ability to serve electronic devices is governed by the energy levels of their molecular orbitals, which can be heavily influenced by functional groups. A convenient method of controlling the behaviour of new π-conjugated materials is the ability to influence a conjugation pathway by facile substitution with various functional groups. Optimization toward the synthesis of these scaffolds has been conducted, and will be discussed. The central focus of this project is to probe the conjugation pathway (red), by variation of R1 and R2, as well as altering the backbone (blue). Similar building blocks show promising optical and electrochemical properties, but are limited in terms of the degree of functionality. This work will demonstrate a synthetic approach that enables fine-tuning of this novel conjugation pathway, followed by investigation of its physical and electronic properties.







Electrolyte and Anode Analysis from Aged Li-Ion Cells

L. M. Thompson[1], M.K.G. Bauer[2], Sam Buteau[2], David Hall[2], L. D. Ellis[1], and J.R. Dahn[1,2]

[1]Department of Chemistry, Dalhousie University
[2]Department of Physics and Atmospheric Science, Dalhousie University

Division: Graduate Materials

Liquid electrolytes are essential to all battery systems, yet little is known of the changes that occur during the lifetime of a cell. It is certain that dramatic changes to the electrolyte of a Li-ion cell occur during operation, because sometimes cells opened at the end of life appear “dry” (i.e. no liquid remaining) even though they were filled with substantial liquid electrolyte upon construction. These electrolyte changes contribute strongly to reducing cell lifetime.

This presentation will discuss the changes to the electrolyte composition during Lithium-ion battery cell life. Data from systematically cycled NMC/graphite cells having various electrolyte compositions and tested at various temperatures and voltages will be included. Results from traditional analysis techniques such as Gas Chromatography-Mass Spectrometry (GC-MS), Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) will be presented with emerging analysis techniques such as Fourier-transformed Infrared spectroscopy (FTIR), and Li-ion cell Differential Thermal Analysis (Li-ion DTA). Observations include increased electrolyte degradation reactions at high upper cut-off voltages as well as increased salt ($LiPF_6$) consumption. The results of these studies indicate the situations where electrolyte degradation is most severe and point to methods to mitigate these problems. These solutions will lead to Li-ion batteries with longer lifetimes.

Synthesis and reactivity of Rh and Ir amido hydride complexes supported by bis(indolylphosphino)silyl pincer ligation

Helia Hollenhorst and Dr. Laura Turculet

Dalhousie University

Division: Graduate Inorganic

The oxidative addition of N-H bonds at late metal centers is a challenging reaction that may offer a pathway to new reactivity for catalytic amination chemistry. Previous work in our group demonstrated that a highly reactive bis(phosphino)silyl iridium species formulated as "(Cy-PSiP)Ir" (Cy-PSiP = □^{3}-(2-Cy$_2$PC$_6$H$_4$)$_2$SiMe) is able to mediate facile N-H bond oxidative addition of ammonia and anilines to afford isolable, terminal amido hydride complexes.[1]Given the rarity of such N-H bond activation reactions, we sought to better understand ancillary ligand effects on metal mediated N-H bond cleavage processes. In this regard, this presentation will detail the synthesis and reactivity of Rh and Ir amido hydride complexes supported by a newly designed bis(indolylphosphino)silyl pincer ligand recently developed in our group.[2]Studies documenting the ability of unsaturated (PSiP)M^{I} (M = Rh, Ir) species featuring such new PSiP ligation to activate the N-H bonds of amines will also be described.

1. Morgan, E.; MacLean, D. F.; McDonald, R.; Turculet, L. *J. Am. Chem. Soc.* **2009**, *131*, 14234-14236.

2. Murphy, L. J.; Hollenhorst, H.; McDonald, R.; Ferguson, M.; Lumsden, M. D.; Turculet, L. *Organometallics* **2017**, *36*, 3709-3720.

Using bipolar electrochemistry to modify glassy carbon with polypyrrole to create supercapacitive materials

Nigel Patterson and Anna Ignaszak

University of New Brunswick, Fredericton

Division: Graduate Materials

Bipolar electrochemistry was applied to create new supercapacitive composite materials from glassy carbon grafted with polypyrrole (PPy). In the first step, a glassy carbon electrode was functionalized with a nitrophenyl linker from the diazonium salt, then reduced to an aminophenyl thin layer. It was found that the addition of this linker layer aided in the mechanical stability of composite, preventing delamination of the PPy layer. PPy was then electrochemically polymerized onto this layer. The composites were characterized by XPS and SEM. The N 1s narrow scans confirm the presence of the desired layer functionality, and therefore successful modification of the electrode surface. SEM and to a lesser extent visual inspection both gave a view of the morphologies of the layers as they were attached to the electrode. Finally, the electrical properties of the composite were characterized as well. The specific capacitance of the composite was found by cyclic voltammetry to be 11 mF/cm^2. Electrochemical impedance spectroscopy showed the PPy layer to be stable around 0.65 V, with degradation occurring near 0.70 V. An Anson plot was drawn from coulometry data to find the diffusion coefficient, 1.2×10^{-11} cm^2/s. Short term charge-discharge of the material through chronopotentiometry found the composite to be stable within the given potential window over the time scale.

A Strong Electron Donor via the Superior π-Electron Donating Ability of a Triphenylphosphonium Ylidyl Group

Morgan Burgoyne, Adam Dyker, Thomas MacDougall, and Zachary Haines

University of New Brunswick, Fredericton

Division: Graduate Inorganic

The π-electron donor strength of a triphenylphosphonium ylidyl group ($Ph_3P=CH$-) was explored through its substitution onto a bispyridinylidene (BPY) scaffold. Electrochemical studies revealed that the triphenylphosphonium ylidyl-substituted BPY is the most reducing di-substituted derivative reported to date ($E_{1/2}$= -1.55 V vs. SCE), which exceeds the reduction potentials of the iminophosphorano counterparts. The utility of this new organic reductant will be exhibited through its use in metal-free reductions targeting new organic substrates. Additionally, by using a previously established correlation,the redox potential of the substituted BPYs allowed for the determination of a Hammett constant for the $Ph_3P=CH$- group (σ_p^+= -2.33), showing it to be the most donating neutral substituent currently known. The information about the donor ability of the methylenephosphorano groups from this study should be broadly applicable and will allow for new and more reducing organic electron donors to be targeted.

A New Method for Determining the Concentration of Electrolyte Components in Lithium-Ion Cells using Fourier Transform Infrared Spectroscopy and Machine Learning

Leah Ellis, Dr. Jeff Dahn, Sam Buteau, Sam Hames, Lauren Thompson, and David Hall

Dalhousie University

Division: Graduate Materials

A new method is introduced for determining unknown concentrations of major components in typical lithium-ion battery electrolytes. The method is quick, cheap, and accurate. Machine learning techniques are used to match features of the Fourier transform infrared (FTIR) spectrum of an unknown electrolyte to the same features of a database of FTIR spectra with known compositions. With this method, $LiPF_6$ concentrations can be determined with similar accuracy and precision as an inductively coupled plasma optical emission spectrometry (ICP-OES) method. The ratios of organic carbonate solvent species can be determined with more rapidity than gas chromatography (GC). This FTIR method is faster and less expensive than GC and ICP-OES, and has the added benefit of being able to determine $LiPF_6$ concentration and solvent fractions simultaneously. Application of this tool can facilitate electrolyte analysis of aged lithium-ion cells, and will help elucidate mechanisms for cell degradation.

Synthesis of Cuprous Oxide (Cu_2O): A Wireless Bipolar Electrochemical Approach

Steven McWilliams and Dr. Anna Ignaszak

University of New Brunswick, Fredericton

Division: Graduate Inorganic

Cuprous oxide (Cu_2O) has been valued and examined extensively due to its high electrical and thermal conductivity[1]; as such, it has been employed for anti-bacterial applications, as supercapacitors and solar cells, for dye degradation, organic synthesis, and as sensors[1]. Cu_2O has been synthesized through various methods including thermal oxidation, electrodeposition, and chemical vapour deposition[1]. However, in previous research, many of these synthesis methods have been argued to be hazardous to the environment due to the choice of solvents (e.g., sodium hydroxide) or the use of copper pre-cursers (e.g., copper sulfate). Furthermore, although the fabrication of Cu_2O has been previously achieved through bipolar means by González Pérez and Bisang[2], it was not considered "green" chemistry. Like that of other environmentally-harmful methods, a caustic solution of sodium hydroxide was utilized during this bipolar fabrication of Cu_2O. Thus, in our research, we have developed the groundwork for a more environmentally-friendly method of Cu_2O synthesis via the use of wireless bipolar electrochemistry. Preliminary results will be presented, and future research directions and possible applications will be discussed.

1. Sun, S.; Zhang, X.; Yang, Q.; Liang, S.; Zhang, X.; Yang, Z. *Journal of Progress in Material Science*, **2018**, 96, 111-173.

2. González Pérez, O.; Bisang, J. M. *Journal of Chemical Technology & Biotechnology*, **2013**, 88, 1314-1320.

Poster Presenters by Division

Analytical

Poster Number	Presenter	School	Division
1	Mary Laeticia Wendy Rose	SMU	Undergraduate
2	Ariana Joseph	SMU	Undergraduate
3	Shruti Bindesri	SMU	Undergraduate
4	Kathleen Allen	SMU	Undergraduate
5	Holly Victoria Barrett	MUN	Undergraduate
6	Gaius St. Marie	SMU	Undergraduate
7	Philip Jakubec	Dal	Undergraduate
8	Katharine Miller	Acadia	Graduate
9	Mimoza Gjelaj	Acadia	Graduate
10	Abdou Ben Ali Adluri	UdeM	Graduate
11	Tyler van de Ven & Efthimios Karmas	Dal	Undergraduate

Biological and Medicinal

Poster Number	Presenter	School	Division
12	Yuriy Barchuk	MSVU	Undergraduate
13	Morgan Crosby	SMU	Undergraduate
14	Guilherme L. Ferreira	MSVU	Undergraduate
15	Kosuke Kanayama	MSVU	Undergraduate
16	Pablo Scrosati	StFX	Undergraduate
17	Alana M. M. Rangaswamy	Dal	Graduate
18	Brendan Grue	SMU	Graduate
19	Julie Anne Dayrit	SMU	Undergraduate

Poster Presenters by Division

Inorganic

Poster Number	Presenter	School	Division
20	Adam Beckett	MtA	Undergraduate
21	Amar Kumar Bhardwaj	UNB-F	Undergraduate
22	Roberto Diaz-Rodriguez	Dal	Undergraduate
23	Livia Ferland	UNB-F	Undergraduate
24	Sydney Hetherington	UNB-F	Undergraduate
25	Meagan Kindervater	MtA	Undergraduate
26	Marcus Kindervater	MtA	Undergraduate
27	Sarah Martell	MtA	Undergraduate
28	Kathleen Morrison	MtA	Undergraduate
29	Maia Murphy & Max Landry	MtA	Undergraduate
30	Ketnavi Ramgoolam	SMU	Undergraduate
31	Jennifer Wright	SMU	Undergraduate
32	Fabien Lindeperg	Dal	Graduate

Materials

Poster Number	Presenter	School	Division
33	Katie Doran	StFX	Undergraduate
34	Govinda Humagain	Dal	Undergraduate
35	Yiqi Lai	Dal	Undergraduate
36	Mollie MacLean	Acadia	Undergraduate
37	Maxine Kirshenbaum	Dal	Graduate
38	Juliana Vidal	MUN	Graduate

Poster Presenters by Division

Organic

Poster Number	Presenter	School	Division
39	Amy Brown	UNB-F	Undergraduate
40	Kalei Crowell	SMU	Undergraduate
41	Jenny Gao-Kang	Acadia	Undergraduate
42	Ryan Hines	SMU	Undergraduate
43	Ryan McCoy	SMU	Undergraduate
44	Jenna McNutt	Acadia	Undergraduate
45	Jun Luo	Acadia	Undergraduate
46	Fanta Ndongou-Moutombi	UdeM	Graduate
47	Jayden T. D. Price	UNB-F	Graduate
48	Melody Yue Shen	Dal	Graduate
49	Waseefa Fatma (no abstract)	Acadia	Graduate
50	Shanghuan Feng (no abstract)	CBU	Graduate

Physical, Theoretical, and Computational

Poster Number	Presenter	School	Division
51	Katherine Budden	SMU	Undergraduate
52	Ian Desmond Conrod	SMU	Undergraduate
53	Isabel S. Curtis	MtA	Undergraduate
54	Alexander Hare	Dal	Undergraduate
55	Felicia Licht	Dal	Undergraduate
56	David Morris	Dal	Undergraduate
57	Alastair J. Price	Dal	Undergraduate
58	Christopher Qiu	MUN	Undergraduate
59	Katherine Reiss	MtA	Undergraduate

Informative Poster

Poster Number	Presenter	School	Division
60	Leah Ellis (Green Chemistry Initiative)	Dal	N/A

Improving Efficiency of Analytical Chemistry using Microwave Digestion

Mary Laeticia Wendy Rose and Mary Sheppard

Saint Mary's University

Division: Undergraduate Analytical

Traditional hot plate digestion of complex samples is time consuming and poses significant safety challenges especially in undergraduate teaching. Three analytical chemistry experiments involving nickel and brass samples were modified to use a commercial microwave digestion system (CEM MARS 6). Microwave digestion decreased reaction time and acid volume up to 92 % and 86 % respectively. Compared to traditional hot plate digestion the accuracy and precision stayed the same. The advantages and disadvantages of microwave digestion compared to traditional hot plate digestion will be presented.

A Laser Polarimeter Laboratory for Measuring Scattering in Undergraduate Analytical Chemistry

Ariana T.K. Joseph, Richard Cisek, Danielle Tokarz, and Katherine Budden

Saint Mary's University

Division: Undergraduate Analytical

This module was designed specifically for third-year undergraduate students to gain first-hand experience in the development of an inexpensive polarimeter from laboratory grade materials. This polarimeter is used in studying light scattering in an aqueous sucrose solution. Additionally, students examine how the polarisation properties of a beam change depending on the type of retarder (quarter-wave plate or half-wave plate) used. The study of polarisation properties is achieved through the measurement of Stokes parameters for calculation of the degree of linear polarization (DOLP). The DOLP calculation serves as a learning tool for students to utilize data verification for production of accurate results. Additionally, students integrate advanced error analysis in the experiment. Surveys taken from students enrolled in the course revealed that the experiment improved their critical thinking skills. In addition to offering the basic skills of beam alignment and polarimeter assembly, it aided in comprehension of course concepts, and improved their research and independent learning abilities.

Development of a Plasmonic Fabric-based Sensor for Point-of-Care diagnostics

Shruti Bindesri, Christa Brosseau, and Dalal Alhatab

Saint Mary's University

Division: Undergraduate Analytical

During the past decade, the demand for modern technologies for point-of-care diagnostics (POC) has increased. This project focuses on developing the next generation sensing platform for rapid and sensitive diagnosis of disease biomarkers in bodily fluids. Textiles are ideal for the design of wearable sensors because of their flexibility and they can be constantly worn without interfering in a person's daily activity. A fabric-based conductive plasmonic sensor was developed from a cotton blend fabric which was used in conjugation with surface enhanced Raman spectroscopy (SERS). The fabric electrodes were first tested using *para*-aminothiophenol (*p*-ATP) as the SERS probe, due to its high Raman activity. Further investigations were carried out to detect levofloxacin in synthetic urine. Levofloxacin is a powerful antibiotic with low clearance rate, used to treat different forms of infections. Detection of this biomarker focused on the use of SERS coupled with electrochemistry (EC-SERS) using the fabric electrodes. The SERS performance of the fabric electrodes was compared with that of the screen printed plastic electrodes that are traditionally used for EC-SERS measurements. This study presents the first use of a low-cost fabric electrode as a SERS substrate with strong enhancement of the analyte signal.

1. Robinson, A, M.; Zhaoa, L.; Yasmina, M.; Bhandarib, P.; Harrouna, S, G.; Dendukurib, D.; Blackburn, J.; Brosseau, C, L. *The Royal Society of Chemistry*, **2012**, 00, 1-3.

Development of a SERS-Based Rapid Vertical Flow Assay for Point-of-Care Diagnostics

Kathleen Allen, Christa L. Brosseau, R. Karaballi, B. Goodall, C. Hui, H. Chan, T. Lynk, and N. Vats

Saint Mary's University

Division: Undergraduate Analytical

Point-of-care (POC) diagnostic testing platforms are a growing sector of the healthcare industry as they offer the advantages of rapid provision of results, ease to use, reduced cost, portability, and the ability to efficiently link patients to care. Chromatographic flow assay technology has been used for many POC testing, however; this technology has several disadvantages such as lack of sensitivity, along with limited capacity for multiplexing and quantitative analysis. Over the last several decades, surface enhanced Raman spectroscopy (SERS) has been used for the detection of biological analytes with high specificity and sensitivity. Coupling SERS with chromatographic flow assay technology will enable on-site acquisition, storage, and transmission of important healthcare metrics. In this work, SERS is coupled for the first time to a rapid vertical flow (RVF) immunotechnology for detection of anti-HCV antibodies. High-quality and reproducible SERS spectra were obtained using gold nanoparticles (AuNPs) that have been modified with *para*-aminothiophenol (*p*-ATP). Many optimization studies such as variation of AuNPs size, *p*-ATP concentration and volume, and monoclonal antibody volume have been conducted to improve the SERS signal. It was observed that increasing the AuNPs size from 13 nm to 30 nm shows drastic enhancement in SERS signal. Also, increasing the volume of the AuNPs added to the RVF test cartridges enhanced the SERS signal and reduced spot-to-spot variation, resulting in increased reproducibility of the test results. A series of dilution studies were conducted that determined the detection limit is 1/2000 diluted antibody.

Development of a Methodology and Apparatus for In Situ Sampling of Polycyclic Aromatic Hydrocarbons in Natural Water Using Molecularly Imprinted Polymers

Holly Victoria Barrett and Dr. Christina Bottaro

Memorial University of Newfoundland

Division: Undergraduate Analytical

Molecularly imprinted polymers (MIPs) are polymers formed in the presence of a template molecule. After polymerization, the removal of the template molecule leaves behind cavities in the polymer whose shape, size, and functionality are complimentary to the template, and hence these cavities can act as highly selective binding sites for specifically targeted analytes.1 MIP formulations using a pseudo-template have been applied for the monitoring of a range of light polycyclic aromatic hydrocarbons (PAHs) in surface waters, as some PAHs are known environmental pollutants and suspected human carcinogens.2 In the presentation, work involving the development of methodologies for the use of PAH MIPs for sampling of a group of six PAH compounds in large volumes of water, as well as the design and production of a sampling apparatus which can be used for in situ deployment in shallow rivers will be presented. This work will examine the advantages of a head space-gas chromatography-flame ionization detection (HS-GC-FID) method for the direct analysis of MIPs to establish a high-throughput methodology that allows for the direct detection and quantitation of PAHs in environmental waters with minimal sample preparation.

1. Beltran, A.; Borrull, F.; Marcé, R. M.; Cormack, P. A. G. TrAC - Trends Anal. Chem. 2010, 29 (11), 1363–1375.

2. Egli, S. N. Thin-Film Molecularly Imprinted Polymers for Detection Systems for Polycyclic Aromatic Hydrocarbons in Water. Ph.D. Dissertation, Memorial University of Newfoundland, 2014.

Novel Ag- Cu Bimetallic Nanostructures for Sustainable Plasmonic Applications

Gaius Justus Hendrickson St. Marie, Christa Brosseau, Osai Clarke, and Jelani Ross

Saint Mary’s University

Division: Undergraduate Analytical

Plasmonics is the field of research which explores the unique optical and electronic effects observed when certain nanoscale metals interact with light. Plasmonic nanostructures that are uniform in size, shape and polydispersity are highly desirable for many applications, including plasmon-enhanced solar cells. Metals which are plasmonic in the visible region include silver (Ag), gold (Au) and copper (Cu). The field of plasmonics is strongly dominated by the use of Ag and Au. Drawbacks to these two metals include high cost and earth- abundance issues in the future. Cu is an excellent alternative metal but suffers from ease of oxidation and a lack of reported nanostructures. In light of this, our focus was to create a novel type of Ag- Cu bimetallic structure which would use much less Ag while maintaining an excellent plasmonic performance as assessed by Surface- Enhanced Raman Spectroscopy (SERS). This work was further applied to investigate the catalytic properties of Cu using EC- SERS (Electrochemical-SERS).

Optimizing sodium dodecyl sulfate depletion via Transmembrane Electrophoresis: Combating Joule Heating

Philip J. Jakubec and Dr. Alan Doucette

Dalhousie University

Division: Undergraduate Analytical

Sodium dodecyl sulfate (SDS) is a widely used surfactant favored for its use in protein extractions, solubilisations, and mass-based separation techniques for proteomic analysis. Surfactants interfere with separation techniques and high-resolution detection methods like liquid chromatography and mass spectrometry (MS). Especially of interest to proteomics is that SDS suppresses MS signals resulting in lower resolution data that makes comparison with bioinformatic databases difficult; so, SDS must be removed from samples prior to MS analysis. Transmembrane electrophoresis (TME) is a recently developed system for protein purification capable of depleting >99% of contaminating SDS, while preserving high protein yield >95%. Increasing the strength of the electric field has proven the key to increasing TME SDS depletion rates, but the resulting increase in Joule heating leads to sample losses. Herein, we optimized the design of the TME device and its procedure to mitigate Joule heating, increasing the rate of sample purification three-fold, while maintaining high sample recoveries. TME is a rapid protein purification technique for the frontend sample preparation of proteomic samples for high throughput MS analysis.

Treatment Efficiency and Stability of Antibiotics in Wastewater

Katharine Miller and Anthony Tong

Acadia University

Division: Graduate Analytical

The presence of antibiotics and other pharmaceuticals in wastewater is a growing concern. In municipal sewage treatment plants (STPs), antibiotics are only partially eliminated and can therefore be discharged into the environment regardless of wastewater treatment, affecting ecological and potentially human health. Target antibiotics in this research included beta-lactams, macrolides, fluoroquinolones, and triclocarban. An analytical method using liquid chromatography – tandem mass spectrometry (LC/MS/MS) was developed for quantifying these antibiotics. The efficiencies of wastewater treatment technologies used in STPs were determined by analyzing antibiotics in wastewater influents and treated effluents. Various treatment technologies were studied, including primary treatment, modified secondary, aerated lagoon, facultative lagoon, sequencing batch reactor, rotating biological contactors, and oxidation ditch. Further, antibiotic stability was investigated for samples stored in three levels of media: ultra-purified water, treated effluent and wastewater. The experiment was carried out under different conditions: in different non-prefiltered or prefiltered with 0.1 µm filters media stored at fridge temperature and room temperature. It was determined that prefiltration of the samples did not markedly affect the stability of the target antibiotics. Temperature was found to have significant impact on the degradation of antibiotics. The half-lives of antibiotics were inversely related to the storage temperature. It was speculated that fluoroquinolones and macrolides have higher persistence suggested by the concentration asymptote creating favouring conditions for the growth of antibiotic resistant bacteria. The activation energies of antibiotic degradation were calculated. High values of activation energies were found, indicating the antibiotic reactivity was mainly affected by the reaction temperature.

Title: Characterization of Nova Scotia Grape and Wine

Mimoza Gjelaj and Anthony Tong

Acadia University

Division: Graduate Analytical

Wine science is based on three distinct pillars: grape culture, wine production and sensory analysis. While understanding of the chemical nature of grapes has developed and advanced significantly worldwide since the early 1900's, the analysis of Nova Scotia grape and wine has seen little to no literary advancements. In this work, Nova Scotia grape and wine samples were analyzed using various analytical techniques including HPLC, UV-Vis Spectrophotometry, flow analysis, and ICP-MS for quantifying organic acids, amino acids, sugars and metals. Further, wines made from the Nova Scotia grape varieties were compared as well as various wines from global regions. Preliminary results of organic acid in grape samples showed highest concentrations of malic, tartaric and citric acids, in a descending order. Sucrose and glucose were found to exist in a 1.25:1 concentration ratio, while fructose showed a 48-time lower concentration compared to glucose. Further, data obtained from ICP-MS analysis indicated highest concentrations of potassium, magnesium and calcium in the grape samples, in the g/L range. Results from these analyses provide insight into each of the three pillars of wine science, contributing to the limited literature with regards to cold climate grapes, in particular, Nova Scotia grape and wine. Through advancing the understanding of the chemical constituents of Nova Scotia grape and wine, and how the climate shapes them, this study will improve vineyard management and wine quality throughout the province.

HPLC-SEC-FTIR characterization of the DOM produced by the microbial carbon pump

Abdou Ben Ali Adluri and Luc Tremblay

Université de Moncton

Division: Graduate Analytical Chemistry

Dissolved organic matter (DOM) represents more than 90% of the organic carbon in the oceans. The microbial carbon pump (MCP) has been proposed as a production mechanism for long-lived DOM. In this concept, microbial activity transforms labile organic matter into more recalcitrant DOM. However, the mechanisms and the molecular transformations involved are mostly unknown. Most characterization techniques require the extraction of DOM which generally discard most of the DOM. New approaches are thus needed. In this study, size-exclusion chromatography (HPLC-SEC), was coupled with Fourier transform infrared spectroscopy (FTIR) by a solvent-elimination interface for the characterization of DOM from natural waters and from incubation experiments. In these experiments, glucose was used as the only source of carbon for natural microbes and the production of more recalcitrant microbial DOM was followed. Before HPLC-SEC-FTIR, the marine DOM was concentrated by evaporation followed by a low elution volume solid-phase extraction (PPL) to avoid DOM losses. Results showed that almost 100% of fresh-water DOM and 80% of seawater DOM were analyzed. During the 1-year incubation experiments, glucose was transformed into more complex DOM. HPLC-SEC-FTIR analyses revealed significant compositional changes with molecular size and origin. These changes may explain the reported contrasting reactivity and fate of different DOM fractions (e.g. small vs large molecules). This study provides a better understanding of the composition of the DOM produced by microbial activity and the MCP.

Development of an Analytical road side test for cannabis impairment

Tyler van de Ven, Efthimios Karmas, and Roderick Chisholm

Dalhousie University

Division: Undergraduate Analytical

With Marijuana becoming legal in Canada, new methods of detecting impairment from the drug must be studied as the current positive/negative test does not account for impairment. Rather the test indicates that the drug was consumed in recent history (the past few days). A struggle in the development of this technology is ensuring that the test is simple and robust, as those that would be conducting the test would not be a chemist. These situations also require detection of impairment compounds rather than simply a positive test for THC. This study aims to create a test where a metabolite of THC is detected in saliva samples. A successful test of this would provide proof of concept in this road side detection technology and aid in the future development of devices to detect if someone is under the influence of marijuana.

The biochemical evaluation of proton pump inhibitors and cholinesterase enzymes

Yuriy Barchuk[1], Sultan Darvesh[1,2,3], Earl Martin[1], and Ian R. Pottie[1,4]

[1]Department of Chemistry & Physics, Mount Saint Vincent University
[2]Department of Medical Neuroscience and the Brain Repair Center, Dalhousie University
[3]Department of Medicine (Neurology and Geriatric Medicine), Dalhousie University
[4]Department of Chemistry, Saint Mary's University

Division: Undergraduate Biological and Medicinal

Background: Proton pump inhibitors (PPIs) are used to treat ulcers in the stomach and relieve symptoms of acid reflux. It has been observed that when people with Alzheimer's disease (AD) take PPIs, their cognitive function improves. AD is the leading cause of dementia worldwide. This disease leads to the reduction of the neurotransmitter acetylcholine in the brain which causes cognitive and behavioural dysfunction. Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), serine hydrolase enzymes, regulate the concentration of acetylcholine within the brain. Known AD therapeutics inhibit AChE and BChE leading to cognitive improvements in AD patients by increasing the amount of acetylcholine. With the observation of improved cognition of AD patients on PPIs, it is hypothesized that PPIs inhibit AChE and BChE, like known AD therapeutics, resulting in higher concentrations of acetylcholine thus improving cognitive function. Biochemical evaluations of known PPIs with AChE and BChE are currently underway.

Methods: Docking studies, using Autodock 4.0, have been performed on 11 reported PPIs to identify sites of interaction between the PPI and each cholinesterase. Pymol software has been used to generated models of this interaction. Enzyme kinetic evaluations are performed with each PPI and selected cholinesterase using a modified Ellman's method.

Results: Completed Autodock calculations show PPIs binding inside of the active site gorge while others bind outside of this key area. Enzyme kinetic evaluations using the modified Ellman's method are now underway.

Conclusion: Docking studies indicated that all 11 PPIs bind to the active site gorge of AChE while 7 of these compounds docked within the active site of BChE. Enzyme kinetics are now underway to validate these data.

Investigation of Microbial Isolates from Nova Scotian Honey Bees as Potential Biocontrols

Morgan Crosby and Clarissa Sit

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Division: Undergraduate Biological and Medicinal

Honey bees are one of the most important pollinators in the agricultural industry. There has been a global decline of honey bees in recent years, with Colony Collapse Disorder (CCD) and American Foulbrood disease (AFB) contributing to this decline. Currently, there are no well-established solutions to either problem. Previous studies suggest that there is potential for microbes isolated from the gut of honey bees to combat the bacterium at the root of AFB, Paenibacillus larvae.[1] We isolated external microbes and internal gut microbes from honey bees that we sampled from several apiaries across Nova Scotia. From these isolates, we extracted metabolites and analyzed them using Reverse-Phase Liquid Chromatography/Mass Spectrometry. These fractions were also tested for general antimicrobial activity, and the most promising samples will be characterized by nuclear magnetic resonances spectroscopy. The isolated microbes will also be tested in a pairwise assay against a commercially available strain of P. larvae. Future plans for genomic sequencing and principal component analysis of metabolites will be discussed.

1. Forsgren, E.; Olofsson, T. C.; Vásquez, A.; Fries, I. *Apidologie*, **2010**, 41, 99-108.

The synthesis and biochemical evaluation of aromatic esters for possible Alzheimer’s disease imaging agents

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Background: Alzheimer's disease (AD) is a neurodegenerative disorder that causes dementia. Symptoms progress over time, becoming severe enough to interfere with daily activities. At present, definitive diagnosis of AD occurs at post mortem via pathology examination of the brain. An accurate, early diagnosis of AD during life could help with disease management and facilitate development of new therapeutics. A characteristic of AD pathology is association with the serine hydrolase butyrylcholinesterase (BuCHE) and radiolabelled agents targeting this enzyme could represent imaging agent for AD diagnosis. Aromatic esters containing a 123-iodine atom have shown promise in AD mouse model experiments as radioligand SPECT imaging agents targeting BuCHE. These compounds could aid in an early diagnosis of AD. To aid in validating that BuCHE is an appropriate biochemical target for an AD imaging agent, a series of iodinated aromatic ester derivatives have been designated for synthesis and biochemical evaluation.

Methods: The synthesis of the aromatic esters can be achieved by mixing the appropriate alcohol and acid chloride in the presence of DBU (1,8-diazabcyclo [5.4.0]undec-7-ene) in a capped reaction vial. Biochemical evaluation of the aromatic ester are now underway to determine the cholinesterase affinity for each compound.

Results: Seven aromatic esters were synthesized in good to low yield.

Conclusions: The aromatic esters have been successfully synthesized and their affinities for cholinesterase are being investigated.

The Development of Butyrylcholinesterase ligands for Diagnosis of Alzheimer's disease

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Division: Undergraduate Biological and Medicinal

Background: Alzheimer's disease (AD) is the leading cause of dementia. At present, diagnosis involves a subjective clinical evaluation of cognitive function and ruling out other causes of dementia. A definitive diagnosis of AD is subsequently achieved by post-mortem examination of the brain, for pathological hallmarks of AD such as β-amyloid (Aβ) plaques and neurofibrillary tangles (NFTs). However, Aβ plaques and NFTs are also found in many cognitively normal older individuals.Early, definitive diagnosis of AD during life could alter disease management and possibly aid in the development of new therapeutics. In AD, there is an accumulation of butyrylcholinesterase (BChE) activity associated with Aβ plaque and NFTs in the cerebral cortex, where normally there is low levels of BChE activity. Therefore, BChE may represent an appropriate biomarker for the development of a diagnosis system for AD.

Methods: The synthesis of targeted iodinated aromatic esters can be achieved by mixing the appropriate alcohol and acid chloride in the presence of triethylamine in a capped reaction vial. The biochemical evaluations can be conducted using UV-vis spectrophotometry.

Results: An iodinated aromatic ester was successfully synthesized. UV-vis repetitive scans showed that it is hydrolyzed by BChE but not by acetylcholinesterase (AChE).

Conclusions: The iodinated aromatic ester was successfully synthesized, and its biochemical evaluation showed it is hydrolyzed by BChE but not by AChE. Continuing work involves kinetic analysis of BChE hydrolysis of the ester and its conversion to ^{123}I-labelled product to assess its ability to act as a possible BChE imaging agent for AD in preclinical analysis.

Quality Determination for Novel Cryoprotectant Development for Cooked Lobster Meat

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Compounds functioning as cryoprotectants found in living organisms protect vital functions of the organism when water freezes into ice. Trehalose has been found to have extensive cryoprotective properties and can be used along with other compounds to preserve cooked lobster meat for preservation in sub-zero conditions for extended periods of time. The aim of this study was to investigate chemical tests that may be used to verify food quality after having been stored frozen for different periods of time. Quality was determined by comparative measures to fresh cooked lobster meat with no cryoprotectant treatment. Salt-soluble protein (SSP) was found to decrease over time. Salt-soluble protein in samples without cryoprotective treatment were found to higher concentrations in SSP over time for a brief period, theorized to be due to the destructive nature of ice formation liberating surface proteins. Thiobarbituric acid reactive substances increased over time, with no significant differences at this point. The chemical measures carried out in this study suggest that simple chemical tests may not be sufficient in determining the quality of a frozen lobster product. Further, morphological tests may be needed to explain the trends observed when conducting the salt-soluble protein tests.

Development of thymidine analogues as inhibitors of Cps2L

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Division: Graduate Biological and Medicinal

Streptococcus pneumoniae is an infectious bacterial strain which has shown high virulence, and resistance towards many antibiotics including penicillin.[1]Cps2L is an enzyme found in *S. pneumoniae*, which is essential to the biosynthetic pathway in building bacterial cell walls. Studies in homologous enzymes such as RmlA have shown that inhibition of the enzyme leads to a marked decrease in virulence and thus pathogenicity of *S. pneumoniae*.[2] The Jakeman group has previously done extensive research towards developing an effective inhibitor of Cps2L, focusing largely on modifying sugars and sugar analogues,[3-5] which act as substrates in the physiological reaction catalyzed by Cps2L (See Figure 1). This project seeks to design and synthesize analogues of thymidine triphosphate (dTTP) as inhibitors, with the intent of improving the fit of the small molecule within the active site of the enzyme. Figure 2 shows two example thymidine derivatives, where the headpiece (phenyl group) may be functionalized in future studies. Synthetic strategies and challenges will be discussed, as well as further variability that may be considered in these structures.

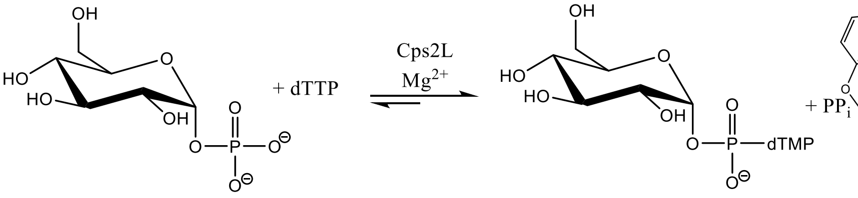

Figure 1. Physiological reaction catalyzed by Cps2L.

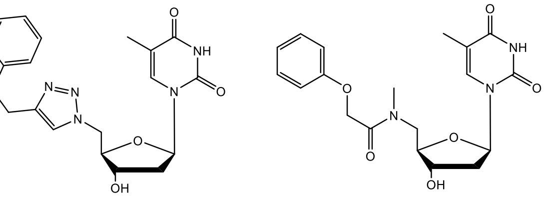

Figure 2. Thymidine derivatives synthesized in this project. The triazole linker (left) and amide linker (right) were determined computationally to improve binding in the active site of Cps2L.

1. Bogaert, D.; de Groot, R.; Hermans, P. W. M. *Lancet Infect. Dis.*, **2004**, 4,144-154.
2. Alphey, M. S.; Pirrie, L.; Torrie, L. S.; Boulkeroua, W. A.; Gardiner, M.; Sarkar, A.; Maringer, M.; Oehlmann, W.; Brenk, R.; Scherman, M. S.; McNeil, M.; Rejzek, M.; Field, R. A.; Singh, M.; Gray, D.; Westwood, N. J.; Naismith, J. H. *ACS Chem. Biol.*, **2013**, 8, 387-396.
3. Forget, S.M.; Jee, A.; Smithen, D.A.; Jagdhane, R.; Anjum, S.; Beaton, S.A.; Palmer, D.R.J.; Syvitski, R.T.; Jakeman, D.L. *Org. Biomol. Chem.*,**2015**, 13, 866-875.
4. Forget, S.M.; Bhattasali, D.; Hart, C.; Cameron, T.S.; Syvitski, R.T., Jakeman, D.L. *Chem. Sci.*, **2012**, 3, 1866-1878.
5. Zhu, J-S.; McCormick, N.E., Timmons, S.C., Jakeman, D.L. *J.Org. Chem.*, **2016**, 81, 8816-8825.

Use of a Polymer-Induced-Liquid-Precursor Process to Induce Intrafibrillar Mineralization in Native Collagen Fibrils

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Previous methods aimed towards the preparation of collagen-based mineralized scaffolds for bone regeneration mainly use methods involving the immersion of randomly oriented collagen fibers in Ca-P containing solutions, such as simulated body fluid (SBF). This research aimed to develop an improved, mineralized collagen-based biomaterial, like that of native bone, that could potentially serve as a regenerative scaffold for bone repair. Specifically, the development of a novel mineralization procedure, including native, aligned, decellularized, and subsequently functionalized collagen fibrils, followed by Mg doped Ca/P alternate soaking mineralization was tested. Additionally, using a polymer-induced-liquid-precursor (PILP) process, it was thought that the prepared mineral phase would remain in an amorphous fluidic state allowing for intrafibrillar collagen penetration before crystal nucleation and growth. Mineralized collagen sheet structure and composition was analyzed through both scanning and transmission electron microscopy (SEM/TEM), energy dispersive X-ray analysis (EDX), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR). Analytical results showed similarities between the prepared scaffold and native bone tissue in terms of both chemical makeup and structural organization. With these results, the prepared mineralized collagen-based scaffold may serve as a possible biomaterial for use towards bone tissue repair systems.

Pairwise testing of *Lentzea* strains against *Mycobacterium smegmatis* to search for new anti-tuberculosis compounds

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Division: Undergraduate Biological and Medicinal

Tuberculosis remains to be one of the top ten causes of death worldwide. Therefore, immediate discovery of new antibiotic compounds is extremely essential for counteracting the evolving antibiotic resistance of strains of Mycobacterium tuberculosis and related species. Previous studies have shown that a soil bacterium, *Lentzea kentuckyensis*, can biosynthesize lassomycin, a peptide that has the ability to kill multi-drug resistant *M. tuberculosis*. Two *Lentzea* strains were grown and observed to have activity against *M. smegmatis*. The active compound was extracted, analyzed, and will be cross-referenced to reported molecules in the literature. Further studies will focus on the investigation of the action of mechanism of the active compound. Novel compounds planned to be characterized will provide a better understanding of how *Lentzea* strains both interact with and defend themselves against competing microbes, such as mycobacteria.

The Synthesis and Characterization of Methylbismuth Dialkoxides as Potential Catalysts for the Ring-Opening Polymerization of Lactide

Adam Beckett and Glen G. Briand

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Division: Undergraduate Inorganic

The emergence of green chemistry can be attributed in part to the breadth of issues associated with the petroleum-based plastic industry.[1]Biocompatible and biodegradable plastics are on the forefront of this field as they address sustainability issues with conventional plastic production.[2] Of these new plastics, perhaps the greatest potential lies in polylactic acid due to its use of renewable feedstocks and biocompatability.[3] The efficient production of PLA, however, requires the use of a Lewis acid catalyst to facilitate the ring-opening polymerization (ROP) of the cyclic dimer, lactide. Previously, one comprehensive study has outlined the potential of single-site bismuth alkoxide complexes as viable catalysts for the ring-opening polymerization of lactide with catalytic activity being notably faster than the industrially standard catalyst, tin(II) octanoate.[4] The goal of this study is to expand upon previous work and synthesize novel methylbismuth complexes supported by {ONNO}-type salen/salan ligands and subsequently screen them for the ring-opening polymerization of lactide. Synthetic approaches, as well as spectroscopic and structural data for isolated compounds, will be presented.

1. A. Sheldon, R. Green Chem. **2017**, 19, 18–43.

2. Kricheldorf, H. R. Chem. Rev. **2009**, 109, 5579–5594.

3. Chen, G.-Q.; Patel, M. K. Chem. Rev. **2012**, 112, 2082–2099.

4. Balasanthiran, V.; Chisholm, M. H.; Durr, C. B.; Gallucci, J. C. Dalton Trans. **2013**, 42, 11234–11241.

Tricyclohexylphosphonium Ylidyl Substituents for a More Powerful Bispyridinylidene Organic Electron Donor

Amar Kumar Bhardwaj, Dr.Adam Dyker, and Morgan Burgoyne

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Ground state organic electron donors and their use as reducing agents have gained more interest and investigation in recent times. More specifically however, it is the fine tunability of these organic reducing agents that is of interest. By modification of substituents on an organic electron donor scaffold such as a bispyridinylidene (BPY), different reduction potentials can be achieved. Previous work with the ylidic triphenyliminophosphorano ($Ph_3P{=}N$-, $\sigma_p^+ = -1.82$) and tricyclohexyliminophosphorano ($Cy_3P{=}N$-, $\sigma_p^+ = -2.21$) substituted BPY's has shown that the group attached to the phosphorous atom has a dramatic effect on the redox potential of the BPY and that the $Cy_3P{=}N$- substituted compound yielded a stronger organic reducing agent ($E_{1/2} = -1.51$V vs SCE). More recently, Dyker and co-workers have found that a triphenylphosphonium ylidyl substituted BPY ($Ph_3P{=}CH$-, $\sigma_p^+ = -2.33$) exceeded the reduction potentials than the iminophosphorano substituted BPY's ($E_{1/2} = -1.55$V vs SCE). This has prompted the synthesis of the related tricyclohexylphosphonium ylidyl substituted BPY ($Cy_3P{=}CH$-), which is predicted to be the strongest disubstituted BPY organic electron donor to date. The synthesis of the tricyclohexylphosphonium ylidyl substituted BPY was attempted and the synthesis and characterization of its direct precursor will be described.

Synthesis and reactivity of aza-dipyrrin alkali metal salts

Roberto Diaz-Rodriguez, Alison Thompson, and Katherine N. Robertson

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Division: Undergraduate Inorganic

Aza-dipyrrins and their derivatives are strong chromophores in the red and near-infrared portion of the spectrum and have wide-ranging applications e.g. as fluorescent probes and sensors, photodynamic therapy agents, and in dye-sensitized solar cells. Because many of these applications employ transition metal complexes of aza-dipyrrins, synthetic methodologies allowing facile and controllable complexation of aza-dipyrrins to metals are valuable. Herein we expand upon previous work from our group[1,2] by reporting the first synthesis and characterization of the alkali metal salts of two representative aza-dipyrrins and detail their use as precursors to some complexes of zinc(II). The lithium salts selectively afford heteroleptic zinc complexes which can be further modified via ligand exchange.

1. Cipot-Wechsler, J.; Al-Sheikh Ali, A.; Chapman, E. E.; Cameron, T. S.; Thompson, A. *Inorg. Chem.* **2007**, *46* (26), 10947–10949.

2. Ali, A. A.-S.; Cipot-Wechsler, J.; Crawford, S. M.; Selim, O.; Stoddard, R. L.; Cameron, T. S.; Thompson, A. *Can. J. Chem.* **2010**, *88* (8), 725–735.

The Uptake of Sterols by β-Cyclodextrin MOFs

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Division: Undergraduate Inorganic

The aim of this project is to create a metal organic framework that may act as a sponge for cholesterol. We have tried to design it to be stable enough to survive in the human body without deteriorating. It was found that a metal organic framework composed of β-cyclodextrin (CD) and potassium can uptake sterols within its pores due to their channel-like structures. Using these sterol-soaked crystals, the MOFs have been analyzed to visually show the channels within the structure as well as interpreted to find the abundance and rate of sterol diffusing out of the pores. Additionally, performing a metal ion exchange with heavier metals (Europium and Terbium) was done to make the crystal structure more stable as well as less soluble in water. They were then analyzed to see if the composition was as expected as well as to find any impurities within the structures.

Towards the Synthesis of Bis(phosphonium ylidyl)ethene Electron Donors

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Division: Undergraduate Inorganic

Recently, it has been demonstrated that bispyridinylidenes with phosphonium ylidic (R_3P=CH-) substituents have higher oxidation potentials than related compounds with ylidic iminophosphorano (R_3P=N-) substituents, allowing for the production of stronger neutral organic reducing agents. Although these compounds are strong reducing agents, they have large molecular weights, which is unfavorable and can complicate purification steps. Based on these considerations, an investigation into R_3P=CH- substituents on a simple and low molecular weight scaffold was conducted. The direct precursors to two compounds, bis(triphenylphosphonium ylidyl)ethene and bis(tricyclohexylphosphonium ylidyl)ethene, were prepared in a single step by the substitution of trans-1,4-dibromo-2-butene with Ph_3P or Cy_3P. Details on the synthesis and characterization of these two precursors, as well as attempts to prepare the bis(phosphonium ylidyl)-substituted ethenes will be presented.

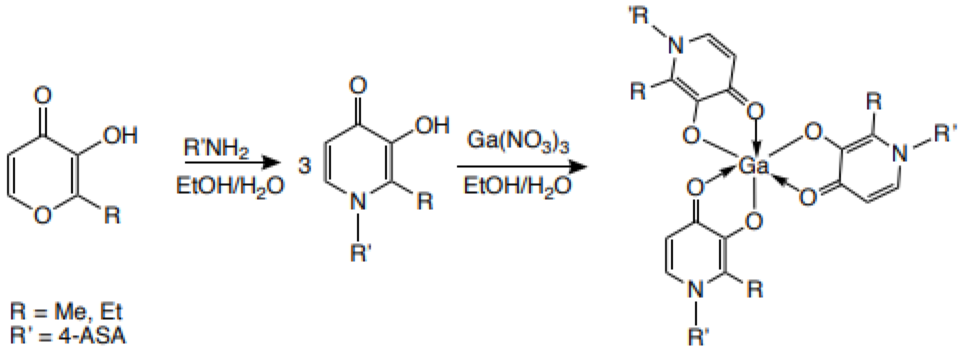
Synthesis of Novel 3,4-Hydroxypyridinones From 4-Aminosalicylic Acid and Their Corresponding Gallium Complexes

Meagan Kindervater, Dr. Stephen A. Westcott, and Christopher Vogels

Mount Allison University

Division: Undergraduate Inorganic

The synthesis of novel metal complexes is an active area of research due to their many possible roles in modern medicine. Much of the motivation into the research of metal complexes can be attributed to the small platinum-based compound, cisplatin. Cisplatin is widely known for its anticancer properties and has become the staple chemotherapeutic. Unfortunately, platinum-based compounds demonstrate drug resistance and toxicity issues. Therefore, non-platinum metallodrugs are being investigated as they do not demonstrate the same horrible side effects. Recently, gallium has demonstrated itself as a promising candidate for new chemotherapies due to its favourable biological effects and anticancer abilities. Notably, 3,4-hydroxypyridinones have been chosen as the preferred ligand due to their capacity to readily deprotonate and accurately deliver and/or remove metal ions from the body. We report thus the isolation of 3,4-hydroxypyridinones synthesized from 4-aminosalicylic acid (4-ASA) and 3,4-hydroxypyrones (maltol and ethyl-maltol) and their subsequent complexation to gallium.



The Preparation of Dinucleating Tetraiminodiphenol Supported Bimetallic Bismuth Complexes and their Potential Application Towards the Ring Opening Polymerization of Lactide

Marcus Kindervater, Glen Briand, and Andreas Decken

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Division: Undergraduate Inorganic

The Principles of Green Chemistry, as outlined by Warner and Anastas in 1998, have encouraged an increased emphasis on sustainability within chemical practices.[1] Significant effort has been invested into biocompatible materials, such as poly(lactic acid), as potential alternatives to traditional petroleum-based plastic production.[2] Poly(lactic acid) is a biorenewable and biodegradable polymer that is efficiently synthesized via the ring opening polymerization (ROP) of lactide, which is facilitated by a metal-alkoxide catalyst. In previous studies, dinuclear aluminum complexes have been shown to efficiently catalyze the ROP of lactide with moderate isotactic selectivity under ambient conditions.[3] This study focuses on the synthesis of a dinucleating macrocyclic N_4O_2tetraiminodiphenol ligand scaffold to support novel bimetallic bismuth compounds. The synthesis and structural characterization of the macrocyclic ligand scaffold and isolated homo- and heteronuclear complexes will be discussed.

1. Anastas, P.; Eghbali, N. *Green Chemistry: Principles and Practice*. *Chem. Soc. Rev.* **2009**, *39* (1), 301–312.

2. Lee, W.-K.; Gardella, J. A. *Hydrolytic Kinetics of Biodegradable Polyester Monolayers.Langmuir* **2000**, *16* (7), 3401–3406.

3. Chen, H.-L.; Dutta, S.; Huang, P.-Y.; Lin, C.-C. *Preparation and Characterization of Aluminum Alkoxides Coordinated on Salen-Type Ligands: Highly Stereoselective Ring-Opening Polymerization of Rac-Lactide.Organometallics* **2012**, *31* (5), 2016–2025.

Investigation of Amine Bis(Phenolate) Supported Bismuth Complexes as Potential Catalysts for the Ring Opening Polymerization of Cyclic Esters

Sarah Martell and Glen G. Briand

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Division: Undergraduate Inorganic

Mass produced petroleum-based plastic materials have become a global issue in terms of renewability, sustainability and disposal.[1] Alternatively, biodegradable plastics such as poly(lactic acid) (PLA), are more sustainable alternatives as they degrade more quickly in the environment and ultimately yield non-toxic and biorenewable materials.[2] The synthesis of polyesters such as PLA is best achieved through ring opening polymerization (ROP) of cyclic esters, which requires a Lewis acid catalyst. These are most commonly metal-alkoxide species which often incorporate toxic metals, such as aluminum and tin.[3]Bismuth-based catalysts offer a greener alternative since the metal possesses low toxicity, is inexpensive, and has minimal environmental impact. The objective of this research is to synthesize and fully characterize novel amine bis(phenolato) bismuth complexes, and to screen these as catalysts for the ROP of cyclic esters, such as lactide. Synthetic methods and spectroscopic data will be discussed.

1. Gross, R. A.; Kalra, B. *Science*, **2002**, 297, 803–807.

2. Gupta, A. P.; Kumar, V. *Eur. Polym. J.*, **2007**, 43, 4053–4074.

3. Balasanthiran, V.; Chisholm, M. H.; Durr, C. B.; Gallucci, J. C. *Dalton Trans.*, **2013**, 42, 11234–11241.

Synthesis, Characterization and Reactivity of (Thiolato)bismuth Lewis Acids

Kathleen Morrison and Glen Briand, Andreas Decken, and Emma D. Smith

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Division: Undergraduate Inorganic

The synthesis and use of catalysts that exhibit low cost and low toxicity to the environment have been an area of increasing interest over the past number of years. Within the last decade, bismuth(III) reagents have been used successfully as catalysts in a variety of organic syntheses [1]. However, the majority of the compounds that have been studied include simple salts, such as triflates, chlorides, and nitrates [2]. We have shown that (dithiolato)indium and -bismuth complexes are water-tolerant and tunable catalysts that may be used as Lewis acid catalysts for esterification and transesterification reactions used in biofuel production [3]. To increase reactivity of these bismuth complexes, we are employing suitable polydentate oxo/aminothiolate ligands that afford (monothiolato)bismuth compounds with increased Lewis acidity but preclude extensive intermolecular interactions. The synthesis and spectroscopic and structural characterization of target compounds along with their screening as water-stable Lewis acid catalysts will be presented.

1. T. Ollevier, *Org. Biomol. Chem.* **2013**, *11*, 2740-2755.

2. B.G.M. Rocha, M.L. Kuznetsov, Y.N. Kozlov, A.J.L. Pombeiro and G.B. Shul'pin, *Catal. Sci. Technol.* **2015**, *5*, 2174-2187.

3. a) G.G. Briand, R. Brüning, A. Decken, M.J. Margeson, H.M. Pickard and E.E. Trevors. *Polyhedron*, **2017**, *135*, 101-108;

   b) G.G. Briand, A. Decken, W.E.M.M. Shannon and E.E. Trevors. *Can. J. Chem.*, **2018**, *e-First Articles*, DOI: 10.1139/cjc-2017-0640.

Schiff Bases, Amino Alcohols, and Boron Salts Derived from Salicylaldehyde Derivatives and Sulfachloropyridazine

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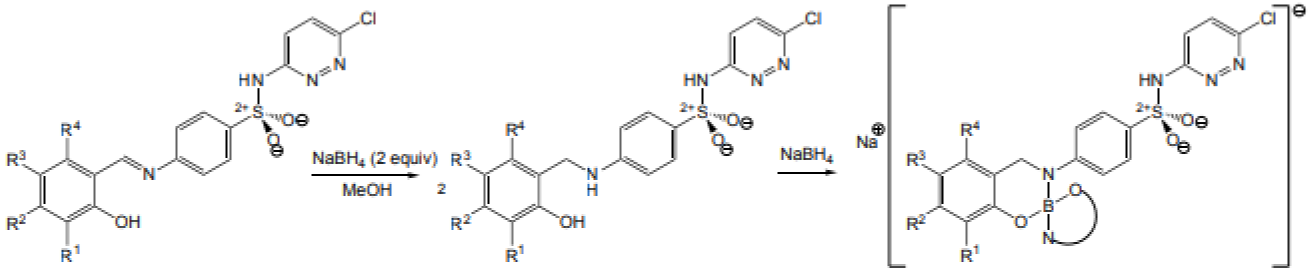
In the past few decades, Schiff bases have gained interest among researchers for their biological properties. These compounds are easy to synthesize and are typically produced from salicylaldehyde derivatives and primary amines. Further, these Schiff bases can be reduced to amino alcohols, many of which also display promising medicinal properties. Elsewhere, organoboron compounds, particularly boronic acids [RB(OH)2] and boronate esters [RB(OR')2], have long been ubiquitous in organic synthesis. Recent research has shown that these same small molecules can display remarkable biological activities. Despite increasing interest in smallmolecule boron pharmaceuticals, relatively little is known about the corresponding boron salts of amino alcohols. Further, variation of both the starting salicylaldehyde and primary amine provides a synthetic strategy that readily allows for the fine-tuning of the physicochemical properties of the Schiff base ligand and hence the corresponding boron salt. We have successfully synthesized a series of six Schiff base ligands by combining various salicylaldehyde derivatives with the antibiotic sulfachloropyridazine. We report herein on our current progress of reducing these Schiff bases to their corresponding amino alcohols by treatment with sodium borohydride (NaBH4). Future work involves synthesizing the four coordinate boron salts by treatment of the amino alcohols with an additional equivalent of NaBH4.



a: R^1=OCH_3; R^2=R^3=R^4=H
b: R^3=Br; R^1=R^2=R^4=H
c: R^1=R^2=R^3=R^4=H
d: R^3=R^4=C_2H_4 (aromatic); R^1=R^2=H
e: R^1=R^3=t-butyl; R^2=R^4=H
f: R^3=F; R^1=R^2=R^4=H

Optimization of the synthesis and purification of [SIPr-H][Cl] (1,3-bis(2,6-diisopropylphenyl) imidazolinium chloride) and new directions in phosphorous chemistry

Ketnavi Ramgoolam and Jason D. Masuda

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Division: Undergraduate Inorganic

Carbenes are molecules that contain carbon centers which are formally two-coordinate and these divalent carbon atoms make carbenes an extremely reactive class of compounds. In 1999, Arduengo reported the synthesis, structure, and characterization of the first stable crystalline carbene.[1] Carbenes can be found in typically two different states namely the triplet state and singlet state and these two states have completely different reactivities. Since the first isolation, their use as ligands in organometallic complexes have become routine. We have been interested in the chemistry and synthesis of carbenes for these very reasons themselves. *N*-Heterocyclic carbenes (NHCs) contain singlet carbeneic carbon centers that are bonded to two nitrogen atoms. In 2008, Robert Grubbs published the article; “*A Facile Preparation of Imidazolinium Chlorides”*.[2] This article describes the preparation of [SIPr-H][Cl] salt involving the reaction of a formamidine with dichloroethane and a base. However, in our hands, this literature method was giving very poor yields (ca. 40%). Therefore, we have developed a new purification method whereby we were able to synthesize the same pure [SIPr-H][Cl] as well as increasing the yield up to 90%.

Sterically bulky substituents are of continued interest due to their ability to stabilize low-valent and low oxidation state main group elements. We have a long-standing interest in phosphorous chemistry and we are currently investigating a series of new redox active compounds. Possible routes to these compounds will be described including our recent progress.

1. Anthony J. Arduengo III, Richard L. Harlow, and Michael Kline, *Journal of the American Chemical Society* **1991** *113* (1), 361-36.

2. Kuhn, K., & Grubbs, R. (2008). A facile preparation of imidazolinium chlorides. *Organic Letters*, *10*(10), 2075-7.

Synthesis of *m*-Terphenyl Substituted Cyclopentadienyl Ligands and Their Metallocene complexes

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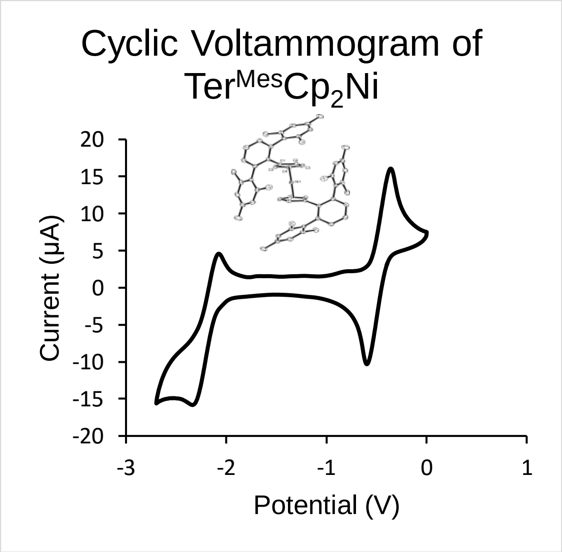
Division: Undergraduate Inorganic

Sterically hindered cyclopentadienyl (Cp) ligands are of continued interest due to their ability to stabilize metal centres. This allows for the isolation of molecules with unusual bonding patterns and reactivity. We have been interested in cyclopentadienyl ligands substituted with sterically encumbered m-terphenyl ligand substituents. These ligands are of particular interest because the aryl groups of the terphenyl can chelate through aryl-pi interactions with the metal center.

A new synthetic route to bulky, more tunable, and chelating cyclopentadienyl ligands featuring *m*-terphenyl substituents was developed, and several alkali metal complexes were prepared and characterised both structurally and spectroscopically.[1] Using structural information obtained from single crystal X-ray diffraction data, it was determined that significant interactions between the flanking aryl groups of the *m*-terphenyl and the metal centres do happen in some cases. Recently, we have prepared three metallocenes, $(^{m\text{-termes}}Cp)_2M$ (.M=Fe, Co, Ni) and their corresponding metallocenium salts. These compounds have been characterized by the normal methods including X-ray crystallography and cyclic voltammetry.



1. Veinot A.J.; Todd A.D.K; Masuda J.D. *A Bulky m-Terphenyl Cyclopentadienyl Ligand and its Alkali-Metal Complexes*. Angew. Chem. Int. Ed. **2017**, 56, 11615-11619.

Iridium mediated P-H bond oxidative addition leading to terminal phosphido hydride complexes

Fabien Lindeperg and Laura Turculet

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Division: Graduate Inorganic

Group 9 metal pincer complexes have shown tremendous utility in a variety of E-H (E = main group element) bond activation reactions. In this context, our group has previously demonstrated that *in situ* generated, 14-electron species of the type (Cy-PSiP)Ir^{I} (Cy-PSiP = $\square^{3}\square(2\text{-}Cy_2PC_6H_4)_2SiMe$) are able to undergo challenging oxidative addition reactions of C-H and N-H bonds.[1] In an effort to further explore the reactivity of such Group 9 silyl pincer species, we focused our recent work on P-H bond activation involving primary and secondary phosphines. Our progress in this direction will be described, including the synthesis and characterization of iridium terminal phosphido complexes. The reactivity of these complexes with respect to P-H reductive elimination, insertion processes, and other reactions with small molecules will also be addressed.

1. Morgan, E.; MacLean, D. F.; McDonald, R.; Turculet, L.; *J. Am. Chem. Soc.* **2009**, *131*, 14234.

Nanoparticle Functionalized Niobium Oxide Perovskites as Visible Light Catalysts for Oxidative Amine Coupling

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Division: Undergraduate Materials

Niobium oxides have gained considerable attention as acid catalysts [1]. Niobium oxide perovskites, such as $KNbO_3$, hold underdeveloped light-activated properties as photocatalysts, in part due to photophysical similarities to more widely studied semiconductor materials, such as TiO_2 [2]. However, perovskites possess inherently larger particle sizes, allowing for facile removal from reaction solutions - highly desirable in heterogeneous catalysis and a key drawback to the use of TiO_2-derived solids. Gold nanoparticle (AuNP) functionalization of $KNbO_3$ provides an opportunity to extent composite response into the visible region through exploitation of the surface plasmon resonance effect [3], in an effort to improve the energetic sustainability of photocatalytic reactions and, specifically, industrially and pharmaceutically relevant organic transformations. In this contribution, we will discuss the experimental procedure for the synthesis and characterization of AuNP/$KNbO_3$hybrids, followed by a systematic study on the use of these materials as possible photocatalysts for the photooxidation of aromatic amines. The influence of aryl substituent and reaction solvent on the overall efficiency of the photocoupling reaction will also be discussed.

1. Nowak, I.; Ziolek, M. *Chem. Rev.* **1999**, *99*, 3603-3624.
2. Shishido, T.; Miyatake, T., Teramura, K., Hitomi, Y., Yamashita, H., Tsunehiro, T. *J. Phys. Chem. C* **2009**, *113*, 18713-18718.
3. Primo, A.; Corma, A.; García, H. *Phys. Chem. Chem. Phys.* **2011**, *13*, 886-910.

Molybdenum Carbide Nanostructures for Efficient Electrochemical Hydrogen Evolution

Govinda Humagain,[1] Kevin MacDougal,[2] Judy MacInnis,[2] Stephanie Macquarrie[2] and Mita Dasog,[1]

[1]Dalhousie University
[2]Cape Breton University

Division: Undergraduate Materials

Hydrogen is the next generation energy source to produce electricity from its stored chemical energy. Sustainable and affordable production of hydrogen is extremely important for extensive commercialization of fuel cells. However, efficiently carrying out the hydrogen evolution reaction (HER) in acidic solution without Pt remains challenging. In the last few years, there has been a concerted effort to develop cheap, active, and stable HER catalysts. Transition metal carbides (TMC) have received considerable attention as alternative electrocatalysts and supporting materials due to either a decrease in the amount of Pt required or in some cases, complete removal of the precious metal. In this study, we show formation of Mo_2C electrocatalysts derived from biochar that shows HER performance similar to Pt metal at 10 mA/cm^2 but better performance at 100 mA/cm^2. The catalysts also showed long-term chemical and mechanical stability. The synthesis of this catalyst is scalable and cheaper than the methods reported previously.

1. Li, J. S.; Wang, Y.; Liu, C. H.; Wang, Y. G.; Dong, L. Z.; Dai, Z. H.; Li, Y. F.; Lan Y. Q.; *Nat. Commun.*, **2016**, 7, 1-8.

Reinventing Porous Silicon Synthesis via Metallothermic Reduction

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[1]Dalhousie University
[2]California Institute of Technology

Division: Undergraduate Materials

Porous silicon is an important nanomaterial with wide applications in drug delivery, gas sequestration, energy storage, and photonics. The utility of porous Si is highly dependent on the surface area, crystallinity, morphology, and pore volume, which are often dictated by the synthetic methods used to prepare them. Over the last 25 years, different methods have been developed for the fabrication of porous silicon, but anodic electrochemical etching of silicon wafers in hydrofluoric acidremains the dominant process. As an alternative to this corrosive process, reduction of silica with metals such as magnesium, aluminum, zinc, etc. has been proposed as a less harmful and scalable pathway. This presentation will focus on preparation of porous silicon by the reduction of silica nanoparticles with magnesium and aluminum metals, a process known as metallothermic reduction. The influence of reducing metals, reaction time, and temperature on the crystallinity, porosity, surface area, and structural integrity of porous silicon nanoparticles will be highlighted. Based on these results, optimum reaction conditions to prepare high-surface area porous silicon will be proposed.

1. Lai, Y.; Thompson, J. R.; Dasog, M. *Chem. Eur. J.*,**2018**, DOI:10.1002/chem.201705818.

Luminescent Properties of "Glow-in-the-Dark" Pigments

Mollie MacLean, Matthew Lukeman, and Marc Hetu

Acadia University

Division: Undergraduate Materials

"Glow-in-the-Dark" products have found a wide variety of uses, particularly in outdoor safety applications, since they can greatly enhance the visibility of people or hazards without the need for electricity. Modern Eu and Dy doped strontium aluminate glow pigments can remain bright for hours after an initial 'charge', although it is desirable to improve both the brightness and longevity of pigments, and to be able to predict their emission properties under a variety of conditions. We have investigated the emission properties of a variety of commercial pigments impregnated in epoxy resins, as well as commercial products containing similar pigments using polyethylene or nylon substrates.

Earth-Abundant Acid-Stable Electrocatalyst for Water Oxidation Reaction

Maxine Kirshenbaum and Mita Dasog

Dalhousie University

Division: Graduate Materials

The oxygen evolution reaction (OER) is an important obstacle to several industrially-relevant processes, including conversion of CO_2 into value-added materials and clean hydrogen production from water-splitting reactions. In electrochemical cells, the OER proceeds more sluggishly than the cathodic reactions, thereby hindering the performance of the overall cell. Many of the electrocatalysts for the OER are unstable under acidic conditions and/or are cost-prohibitive for large-scale application.[1] Thus, efforts are being made to develop economic and sustainable OER electrocatalysts from Earth-abundant materials.[1-5] Herein, we report the discovery of a material with the lowest overpotential in relation to all other cited Earth-abundant materials. Titanium diboride (TiB_2) was found to have an overpotential of 640 ± 80 mV. Elemental analysis was performed on the electrolyte and electrode materials before, during and after water electrolysis using inductively coupled plasma mass spectroscopy (ICP-MS), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). Electron microscopy was performed on films prior to electrocatalysis to assess film surface and thickness.

1. McCrory, C. C. L. *et al. J. Am. Chem. Soc.* **2015**, *137*, 4347.

2. Roger, I.; Shipman, M. A.; Symes, M. D. *Nature Reviews Chem.*, **2017**, *1*, 0003.

3. Yin, Q.; Hill, C. L. *Nature Chem.* **2018**, *10*, 6.

4. Moreno-Hernandez, I. A. *et al. Energy Environ. Sci.*, **2017**, *10*, 2103.

5. Blasco-Ahicart, M. *et al. Nat. Chem.* **2018**, *10*, 24.

Biochars as catalysts for the synthesis of cyclic carbonates from carbon dioxide and epoxides

Juliana Vidal, Stephanie MacQuarrie, and Francesca Kerton

Memorial University of Newfoundland

Division: Graduate Materials

Due to environmental concerns, the development of efficient procedures for the modification, capture and storage of greenhouse gases has grown in importance. Carbon dioxide (CO_2) is a non-toxic, readily available and inexpensive feedstock for the synthesis of industrially important chemicals.[1] An important example of CO_2utilization is its reaction with epoxides to produce cyclic carbonates, which can be used as polar aprotic solvents, electrolytes for batteries, and intermediates for pharmaceutical products.[2] Biochar obtained via biomass pyrolysis under a limited supply of oxygen at low temperatures can be considered a sustainable source of carbon,[3] which has potential as a catalyst support. Because of its inherent easily tuned surface functionality and porosity, biochar can be applied directly as a catalyst or it can be used as a platform for the synthesis of other functional materials.[3] In this work, we report the use of oxidized biochar as a catalyst for the synthesis of cyclic carbonates from CO_2 and epoxides. The reaction parameters were optimized to achieve the highest conversion using the mildest possible conditions.

1. Liu, Q.; Wu, L.; Jackstell, R.; Beller, M. *Nature Communications*, **2015,** 6, 5933.

2. Martín, C.; Fiorani, G.; Kleij, A. W. *ACS Catalysis*, **2015**, 5, 1353.

3. Liu, W. J.; Jiang, H.; Yu, H. Q. *Chemical Reviews*, **2015**, 115, 12251.

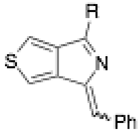
Synthesis and Functionalization of Thienopyrrole Derivatives

Amy Brown and Dr. Sara Eisler

University of New Brunswick, Fredericton

Division: Undergraduate Organic

Thienopyrrole derivatives can be used as small, organic building blocks for synthesis of larger π-conjugated systems. The goal of this project is to determine an optimized synthetic route of functionalized thienopyrrole scaffolds (compound **1**), where R can be a variety substituents, incorporated by cross-coupling reactions. The investigation of the electronic and physical properties of these thienopyrrole derivatives by UV-Vis, fluorescence, and cyclic voltammetry will be discussed.



1

Liquid Assisted Grinding (LAG) for the *N*-Demethylation of Alkaloids

Kalei Crowell and Robert D. Singer

Saint Mary's University

Division: Undergraduate Organic

Within the first decade of the twenty first century the opioid crisis has grown, thus increasing the number of opioid overdoses around the world. This has created a need for the synthesis of drugs that can combat drug overdoses. Previous research aimed at addressing this has focused on using a modified version of the Polonovski reaction for the *N*-demethylation of an *N*-oxide hydrochloride salts of a series of alkaloids. The *N*-demethylation of dextromethorphan, DXM, has been catalyzed using iron (0), Fe^0, both from activated iron (0) dust and nanoscale zero valent iron particles, nZVI. Initial optimization of the reaction demonstrated the use of nZVI in green solvents. Recently, further improvement of this system was demonstrated using **L**iquid **A**ssisted **G**rinding Syntheses (LAG-synthesis). Further improvements utilizing other iron sources and using LAG-synthesis in preliminary steps of the overall synthetic sequence will be discussed.

Towards the synthesis of 5,13b-dihydro-9H-benzo[1,2]indolizino[7,8-b]indole-6,9(7H)-diones as alkaloid analogs

Jenny Gao-Kang, Amitabh Jha, Mukund P. Tantak, Angela Kaiser, Miranda Walsh, Denver Gilbert, and Rebecca Strachan

Acadia University

Division: Undergraduate Organic

Fused heterocycles, such as benzoindolizines and beta-carbolines are found in many natural products and biologically active molecules. We have envisaged the synthesis of 5,13b-dihydro-9H-benzo[1,2]indolizino[7,8-b]indole-6,9(7H)-diones from natural amino acid-based phthalimides and substituted indoles through a sequence of reduction and two successive electrophilic aromatic substitution reactions. The results obtained thus far will be presented.

Synthesis of Cu(II)-NHC complexes in air using 1,3-bis(pyridylmethyl)imidazolium ligands

Ryan Hines, Robert D. Singer, and Daniel O'Hearn

Saint Mary's University

Division: Undergraduate Organic

Copper *N*-heterocyclic carbene complexes (Cu-NHCs) are prevalent in the literature and their stability and catalytic activity is well characterized and established. In an overwhelming majority of reported examples, copper is present as Cu(I) while there are very few reports of Cu-NHCs containing Cu(II). The synthesis and characterization of two air and moisture stable Cu(II)-NHC complexes by direct combination of 1,3-bis(pyridin-2-ylmethyl)-1*H*-imidazolium chloride with copper(II) hexafluorosilicate will be presented. The design of related ligands and their use in the formation of Cu(II)-NHCs and ionic **M**etal **O**rganic **F**rameworks (MOFs) will be discussed.

A Spectroscopic Investigation of the Rhodium-Catalyzed [5 + 1 + 2 + 1] Cycloaddition of Vinylcyclopropanes, Terminal Alkynes and Carbon-monoxide

Ryan McCoy, Kai Ylijoki, and Ifenna Mbaezue

Saint Mary's University

Division: Undergraduate Organic

Spectroscopic investigations on the $[RhCl(CO)_2]_2$catalysed [5 + 1 + 2 + 1] cycloaddition of 1-(2-methoxyethoxy)-1-vinylcyclopropane (VCP), CO, and 4-ethynylbiphenyl were performed and an off-cycle species was revealed. This species, with a determined crystal structure, forms at high Rh-catalyst loading and mitigates cycloadduct formation. Increased temperatures and longer reaction periods did not overcome the action of this species. The starting material for the spectroscopic study, VCP, was synthesised by modifying a procedure from Wender *et al.*[1] The reaction of N-bromosuccinimide with 2-methoxyethanol and 1,3-butadiene in toluene resulted in a brominated intermediate. Purification of the intermediate by column chromatography followed by an elimination reaction afforded 2-(2-methoxyethoxy)-1,3-butadiene, which was subsequently purified by a modified vacuum distillation method. TLC monitored Simmons-Smith cyclopropanation was performed on the diene, resulting in VCP, which was also purified by the same method employed for the diene. IR spectroscopy was performed on mixtures of the cycloaddition reactants, with future work being to monitor the carbonyl peaks *in situ* in an effort to learn more about the kinetics of this reaction and to extract a rate law.

1. Wender, P. A.; Dyckman, A, J.; Husfeld, C. O.; Scanio, M. J. C. *Org. Lett.* **2000**, 2, 1609.

Excited State Proton Transfer Reactions in Polyaryl Phenols

Jenna McNutt and Matthew Lukeman

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Division: Undergraduate Organic

Electronic excitation of phenols can cause them to become more acidic by several orders of magnitude, and in some cases, can cause the phenolic proton to transfer to basic sites on the same molecule, to produce a phototautomer. These reactions can be very fast and efficient, and have been exploited in the design of sunscreens and laser dyes. In molecules where the basic site is a carbon atom, the phototautomer produced is known as a quinone methide (QM). QMs can subsequently undergo reverse proton transfer, electrocyclization, or addition reactions. It is believed that the most efficient examples of proton transfer to produce QMs require a highly polarized excited state. We are testing this claim by synthesizing highly symmetric polyaryls with two phenol residues, and studying their photochemical reactivity.

Green synthesis of novel heterosteroids for 2-aminonaphthalenes

Jun Luo, Waseefa Fatma, and Amitabh Jha

Acadia University

Division: Undergraduate Organic

Synthesis of structurally complex molecules in a short route from readily available starting materials is a challenge in organic synthesis. Therefore, multistep reactions in a domino fashion are being widely investigated by organic chemists. Polyheterocyclic frameworks are very important moieties for the construction of biologically and pharmaceutically relevant molecules. We have developed a highly efficient, transition metal-free, cascade reaction of 2-amino-1-hydroxymethylnaphthalines or 2-amino-1-carboxy-naphthalenes with oxo-acids to produce tetracyclic heterosteroidal framework. It involves one-pot formation of an amide bond, a C-N bond and a C-O bond in tandem. The results obtained thus far will be presented.

Investigations of new green catalytic hydrogenations of pinenes

Ndongou-Moutombi Fanta, Mohamed Touaibia, and Mohamed Touaibia

Université de Moncton

Division: Graduate Organic

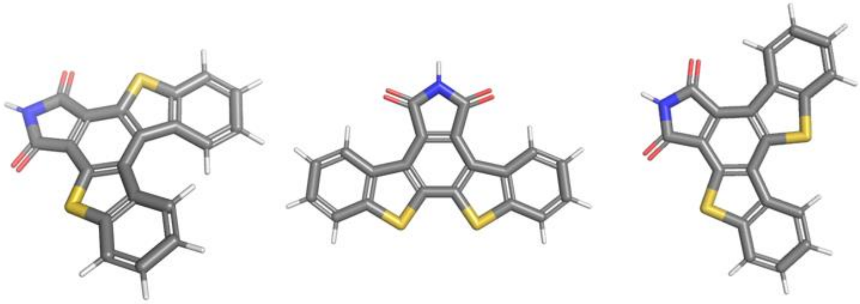
Nowadays, value-added natural products are of great interest in organic synthesis, which justifies the importance of investigating new methods, particularly green ones for their synthesis. Thereby a facile method of selective pinene hydrogenation has been investigated over platinium, ruthenium and rhodium on different supports using green conditions. Reaction time, temperature, catalyst support as well as the transition metal were the different parameters investigated in those reactions. Therefore, our results show that the hydrogenation of α-pinene over ruthenium on charcoal as support with sonication at room temperature leads to a quantitative conversion to pinanes with a highly selectivity in favor of the *cis*-pinane. The same result was obtained for hydrogenation of β-pinene with ruthenium over alumina without sonification at room temperature. The Ru/C has been recycled and reused six times with a constant conversion, catalytic activity and selectivity in favor of *cis*-pinane.

Dibenzothienoisoindole dione D-A type organic building blocks

Jayden T.D. Price, Emily Albright, and Sara Eisler

University of New Brunswick

Division: Graduate Organic



Donor-acceptor (D-A) type organic building blocks are currently being pursued as active components to enhance efficiency in various organic electronic devices (OEDs). This work explores the synthesis, derivitization, and characterization of a series of new isomeric D-A type building blocks, composed of maleimide (acceptor) and benzothiophene (donor) moieties, for application in OEDs. With these modifiable scaffolds, properties desirable for commercial applications may be incorporated, such as increased charge mobility and power-conversion efficiency, enhanced thermal, electronic and optical stability, strong light absorption across a broad range of wavelengths, and improved processability. Computational analysis of the target compounds, as well as their optical and electronic properties, will be presented.

Construction of aromatic heterocycles using “non-precious” metal catalysts

<u>Melody Yue Shen</u> and Gregory Dake

Dalhousie Unviersity

Division: Graduate Organic

Investigations of cross-coupling/condensation processes catalyzed by nickel or copper salts to form aromatic heterocycles such as indoles or azaindoles will be presented.

Nonlinear Optical Second Harmonic Generation Polarimeter Calibration

Katherine Budden, Danielle Tokarz, Ariana T.K Joseph, and Richard Cisek

Saint Mary's University

Division: Undergraduate Physical, Theoretical, and Computational

Nonlinear polarimetry is a non-invasive, non-destructive technique for measuring nonlinear optical activity in diverse organic or inorganic substances. It includes frequency mixing processes, such as second or third harmonic generation. Polarisation nonlinear microscopy is a potential form of recognizing disease development during patient treatment. Although effective for differentiating pathology samples, it is a lengthy process, and is limited to a single wavelength. We are developing a new technique, structural measurement via optical microscopy, that will perform live scans ~1000x faster than previously performed. This will be achieved by developing a multi-spectral nonlinear polarimeter based on photoelastic modulators. However, a complete set of polarization states is required to achieve the nonlinear polarimetry, which is difficult to obtain rapidly. For modeling, a Python program was written to simulate polarization light parameters obtained when a laser beam passes through optics. The program was used to identify the ideal photoelastic modulator (PEM) settings to optimize nonlinear polarimetry. The ideal optical system consisted of two PEMs in series, the first at 45° and the second at 0°, with a phase modulation of 2 and , respectively. In this configuration all possible polarisation states could be obtained. A 3D Poincare sphere was utilized for visualization and evaluation of the polarization states. The simulation showed an even distribution of polarisations using this visualization method, allowing for optimum choice of polarizations states for nonlinear polarimetry.

Crystallization Studies of a Deep Eutectic Solvent

Ian Desmond Conrod and Dr. Kathy Singfield

Saint Mary's University

Division: Undergraduate Physical, Theoretical, and Computational

Differential scanning calorimetry (DSC) and hot stage polarized-light optical microscopy (PLOM) were used to study the isothermal melt-crystallization kinetics and melt behaviour of a deep eutectic solvent (DES) system. The DES in this study is a binary system of choline chloride and urea. The two solids are mixed to form a liquid at room temperature. The eutectic composition is 67 mole% urea. The DES was crystallized isothermally at different temperatures in the range of -40°C and -10°C. The heat flow data from DSC and the total depolarized light intensity signal from PLOM were each subjected to Avrami kinetics treatment. The maximum crystallization rate was found to occur at -20°C. The value of the Avrami exponent indicated a two-dimensional disc growth habit for the DES crystals.

Comparison of the effects of fine-tuning the interfacial tension vs. mediating interparticle interactions on nanoparticle self-assembly at oil/water interfaces

Isabel S. Curtis, Yuwei Zhang, and Dr. M. Vicki Meli

Mount Allison University

Division: *Undergraduate Physical, Theoretical, and Computational*

The preparation of two-dimensional thin films from nanoparticles has been an attractive topic with potential to affect a broad variety of applications in biomedical and materials applications due to their interesting electronic, optical, and mechanical properties. Self-assembly of gold nanoparticles, whose properties depend strongly on their distance from neighboring nanoparticles, is an attractive method to enable the control of nanoparticle packing due to its scalability and reversibility. The interfacial self-assembly of small (<5 nm core diameter) nanoparticles is problematic however, due to the competing effects of the thermal fluctuation energy. Previously, we have found that interfacial films of gold nanoparticles of ca. 2.5 nm average diameter can be formed at some oil/water interfaces using mixed ligand shells consisting of both OH- and CH_3-terminated thiols, as well as vigorous shaking/emulsion formation. We have found that both the interfacial free energy and the nature of the additives/dispersing agent can have a significant effect on the interfacial nanoparticle assembly, and the apparent film properties. Comparison between a series of n-alkane/water interfaces as well as comparison between dispersing agents ethanol, n-butanol and t-butanol will be discussed.

The impact of carbon surface oxides on self-discharge in acidic-aqueous-electrolyte electrochemical capacitor electrodes

Alexander Hare and Heather Andreas

Dalhousie University

Division: Undergraduate Physical, Theoretical, and Computational

It is well known that when oxidized, carbon electrochemical capacitor (EC) electrodes form a variety of carbon oxides, such as quinones, lactones, ethers, and carboxylic acids. While some improve capacitance (e.g. pseudocapacitive quinone groups), the impacts that these surface functionalities have on carbon self-discharge is not understood. This project studies the impacts of oxygen surface functionalities on the self-discharge of four carbon powders: Vulcan XC72, pristine birch biochar, HNO_3-oxidized biochar, and KOH-oxidized biochar. It is extremely important to develop an understanding of self-discharge mechanisms for ECs because it allows for the development of preventative measures that stop self-discharge from occurring, enabling the development of more efficient and reliable charge storage devices. To study the effect of oxidation on self-discharge, cyclic voltammetry (CV) and open-circuit potential self-discharge measurements were run in 1 M aqueous H_2SO_4 electrolyte. X-ray photoelectron spectroscopy (XPS), thermally programmed desorption (TPD), and CV were performed in order to determine degree and type of oxidation. Comparison is made between the self-discharge of each carbon material before and after oxidation through repeated CV cycling, as well as between the first and last charge/self-discharge cycles. It has been shown that self-discharge decreases for all carbons as self-discharge cycling repeats. Fully oxidizing Vulcan is shown to have a minor impact on its self-discharge. Fully oxidized KOH-oxidized biochar showed less self-discharge compared to its as-received state. Pristine birch biochar was found to be a poor EC, and self-discharge for HNO_3-oxidized biochar showed little change, likely because its surface was already fully oxidized.

The Impact of Electrode History on the Coulombic Efficiency of Manganese Oxide Films with Varying Degrees of Hydration

Felicia Licht and Dr. Heather Andreas

Dalhousie University

Division: Undergraduate Physical, Theoretical, and Computational

Manganese oxide is a pseudocapacitive material, storing charge via fast, reversible redox reactions. Ideally, the amount of charge delivered from the pseudocapacitive material is equal to the amount of charge stored; a ratio called the coulombic efficiency (CE). Unpublished work of the Andreas' lab has demonstrated that when multi-current GCD is performed on manganese oxide films, the lower currents resulted in CEs exceeding 100% following higher currents, which is theoretically impossible. The goal of this project is to examine manganese oxide films to determine if the electrode history, film hydration and rate at which the film is charged and discharged impacts the measured CE. Single-current GCD was performed on manganese oxide films to eliminate and test the effects of electrode history. CEs of single-current GCD were significantly lower than 100%, indicating that electrode history is affecting the measured CE. A transmission line circuit (TLC) is a hardware circuit that was used to confirm the occurrence of charge redistribution (CR) within the films. The TLC results also mirror manganese oxide films in that the CE of cycle one was significantly lower than the proceeding cycles which climbed to higher CEs. This indicates that CR significantly occurs in the first GCD cycle and charge is then retained in the bulk film. CR also occurs more in hydrous films as charge can migrate deeper into the bulk compared to heat-treated films. Finally, in proceeding cycles, the CE climbed to 100% as a CR equilibration was achieved between the bulk and active film.

X-ray spectroscopy studies of $Au_{38}(SR)_{24}$ nanoclusters

David Morris[1], Peng Zhang[1], Tatsuya Higaki[2], Rongchao Jin[2]

[1]Department of Chemistry, Dalhousie University

[2]Department of Chemistry, Carnegie Mellon University, Pittsburgh, U.S.A.

Division: Undergraduate Physical, Theoretical and Computational

Gold nanoclusters (NCs) with protective thiolate ligands have emerged as a species of great scientific interest due to their high stability and precisely controlled composition, making them an ideal candidate for various applications. To better understand the structure and properties of these nanoclusters, a technique known as extended X-ray absorption spectroscopy fine structure (EXAFS) is used to provide information on parameters such as the coordination number and bond distance for specific atoms in a nanocluster. The well-known $Au_{25}(SR)_{18}$ nanocluster is first studied to provide a baseline for comparison with the more complex $Au_{38}(SR)_{24}$ nanocluster, with the goal of determining how structural parameters of the nanoclusters vary with changing temperature. Through fitting of the experimental data, it was determined that the synthesized $Au_{38}(SR)_{24}$ nanocluster experiences no change in bond length as temperature is increased, a result differing from the $Au_{25}(SR)_{18}$ NC which experiences an increase in bond length as temperature is increased. The results from EXAFS analysis on the two nanocluster systems studied in this project show the usefulness of theoretical and experimental EXAFS methods in probing the NC structure and bonding properties. Results on the $Au_{38}(SR)_{24}$ NC provide some new findings to help better understand the temperature-dependent properties of $Au_{38}(SR)_{24}$.

Dispersion-Corrected Density-Functional Theory Applied to Amino-Acid Adsorption on Model Quartz Surfaces

Alastair J. Price and Erin R. Johnson

Dalhousie University

Division: Undergraduate Physical, Theoretical, and Computational

Controlled growth of enantiopure biomolecules is an important area of development for modern chemistry. Hydroxylated quartz surfaces are chiral surfaces with many possible hydrogen bonding sites, making them potentially promising substrates to seed enantiospecific separations. We extend the current understanding of the interaction of amino acids with this surface, focusing on alanine, serine, and aspartic acid. Dispersion-corrected density-functional theory (DFT) was used, specifically the B86bPBE functional [1,2] with the exchange-hole dipole moment (XDM) dispersion model [3]. This work can be used as a stepping stone to provide further insight into how amino acid crystals will interact with this surface.

1. Becke, A. D. *J. Chem. Phys.* **1986**, 85, 7184.

2. Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, 77, 3865.

3. Otero de la Roza, A.; Johnson, E. R. *J. Chem. Phys.* **2012**, 136, 174109.

Computational Study of Tetrabenzocoronene Derivatives

Christopher Qiu, Yuming Zhao, and Christopher Flinn

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Division: Undergraduate Physical, Theoretical, and Computational

Tetrabenzocoronenes (TBCs) are polycyclic aromatic hydrocarbons (PAHs) with intriguing structural and photophysical properties. This presentation describes a computational study of TBCs with substituents such as fluorine, chlorine, hydroxide, methoxy, amine, and nitrile groups in the 4,5,14,15 positions (i.e., the “cove region”) based on density functional theory (DFT) calculations. TBCs with these substituents in the 2,7,12,17 positions were also investigated and compared to the “cove” substituted TBCs. The geometries and energies of the TBCs were first optimized and calculated at the group state, as well as the transition state to evaluate the energy barriers for the isomerization between different possible stereoisomers. The frontier molecular orbitals (FMOs) were also examined to determine the electronic properties of the different TBCs. Nuclear magnetic resonance (NMR) calculations were performed to determine the effect of substitution on the aromaticity of the delocalized system. Time-dependent density functional theory (TD-DFT) calculations were also performed to simulate circular dichroism spectra and determine electronic properties. The results of this study indicated that the geometries of “cove” and “non-cove” substituted TBCs varied due to the steric effects of the substituents and that the energy barriers are significant for the interconversion between the *cis* and *trans* isomers so that they can exist distinctly at room temperature.

Investigating the Effects of Gold Nanoparticle Core Size on Ligand Number Density, Phase State, and Mixing

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The study of self-assembling gold nanoparticles is of great interest due to the unique and often size and shape-dependent electronic, physical and optical properties of the nanoparticles. In general, the mixing of nanoparticles with other media is poorly understood. This is in large part due to the immense synthetic possibilities that allow for variability in nanoparticle sizes and shapes, and the implications this has on the ligand caps—the frontline in nanoparticle mixing. Currently, both ligand density and phase have been shown to have surprising effects on nanoparticle-nanoparticle and nanoparticle-solvent interactions.[1]Although the ligand number density on the nanoparticle surface can be adjusted by choice of the ligand binding motif, the consequent effects on ligand dynamics and phase properties are poorly understood. In this study, a series of nanoparticle core sizes are synthesized in order to investigate the resulting effects on ligand density and mixing with secondary components (solvents). To vary surface curvature we have begun to synthesize a series of spherical gold nanoparticles with core diameters from 5 – 40 nm according to the established synthetic procedure by Jana *et al.*, followed by ligand exchange for a hydrophobic alkanethiol ligand.[2] UV-vis spectroscopy is being used to track the ligand exchange process and analyzed using a re-parametrized DLVO-based model by Wijenayaka *et al.* to more accurately assess the nanoparticles.[3] X-ray photoelectron spectroscopy will also be used to determine the thickness of the ligand layer. FT-IR spectroscopy of 5nm particles mixed with deuterated alkanes to assess the phase state of the ligand shell will be presented, and applied to the current study.

1. Boles, M. A.; Engel, M.; Talapin, D. V. *Chem. Rev.*, **2016**, *116*, 11220-11289.

2. Jana N. R.; Gearheart, L.; Murphy, C. J. *Langmuir*, **2001**, *17*, 6782-6786.

3. Wijenayaka, L. A.; Ivanoc, M. R.; Cheatum, C. M.; Haes, A. J. *J. Phys. Chem.*, **2015**, *119*, 10064-10075.

Promoting Green Chemistry at Dalhousie

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Green chemistry is the discipline of chemistry concerned with minimizing hazards and hazardous substances in chemical processes. Practicing green chemistry involves analyzing and evaluating the methods used in a given chemical procedure with the aim of reducing their hazard and environmental impact. The Green Chemistry Initiative is a student-led group looking to increase awareness of the principles of green chemistry 1 and promote the implementation of safe and more sustainable practices in chemistry and other areas of science. This poster provides an overview of green chemistry, our society and contributions, and actionable items for the community. Our membership spans the undergraduate, postgraduate, postdoctoral, and faculty levels of the Dalhousie University Department of Chemistry. We are looking to expand to new departments and universities.

1. Anastas, P. T.; Warner, J. C. Green Chemistry: Theory and Practice, Oxford University Press: New York, 1998.