

2010 WNY ACS Undergraduate Research Symposium



The 2010
Undergraduate Research Symposium

Sponsored by the Western New York Section
of the American Chemical Society

and by

the Student Affiliates of the ACS, Niagara University Chapter

Saturday March 6, 2010

Niagara University, NY



Welcome to the Undergraduate Research Symposium!

The organizers and sponsors of this symposium are thrilled to convene this informal gathering, which, nonetheless, is a great opportunity to get a taste of the research efforts going on in Chemistry fields in our area. For students, this is chance to show off your efforts and see a little bit of how scientists traditionally interact. For faculty members, it's good to be able to shake off some of the moss and ivy and get to know colleagues from other area programs. We welcome participants from across New York State as well as Ontario, Canada. In addition, we are pleased to have Dr. Ignacio Baca from the Department of Chemistry at McMaster University and Dr. Susan Burke from Bausch and Lomb give the keynote addresses.

Sincerely,

Ronny Prierer
Chair, 2010 Symposium Committee

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2010 Undergraduate Research Symposium

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Schedule of Events

Saturday, March 6, 2010

8:30-9:00 am	Registration / Poster setup / Coffee
9:00-10:00 am	Keynote presentation by Dr. Susan Burke Bausch and Lomb “Chemistry of Vision Care Technologies”
10:10-11:50 pm	Student oral presentations (4 X 25 minutes) (Vini 301 and Vini 315)
12:00-1:00 pm	Lunch
1:00-2:00 pm	Student Poster Session
2:05-3:05 pm	Keynote presentation by Dr. Ignacio Baca McMaster University “Supramolecular Main-Group Chemistry: From Fundamental Bonding Studies to Functional Materials”
3:05-3:15 pm	Symposium Awards and Closing Remarks

Our Keynote Speakers



Born in Mexico City, Dr. Ignacio Vargas received his early chemical education at the Chemistry Faculty of the National Autonomous University of Mexico (UNAM). During this period he carried out synthetic and kinetic studies of transition metal coordination complexes under the direction of Lena Ruiz-Azuara. His achievements earned him the Gabino Barreda silver medal, UNAM's most prestigious student award, for each of his undergraduate and Master's degrees. Sponsored by UNAM, he pursued doctoral studies at the University of Calgary, Alberta, Canada, working with Organo-Chalcogen-Nitrogen systems under the supervision of Tristram Chivers and the advice of Tom Ziegler on theoretical studies. After receiving his Ph.D. degree, he moved to Montreal to investigate nonlinear optical materials with Mark P. Andrews at McGill University, in collaboration with Mark Kuzyk at Washington State University. Ignacio Vargas later moved to the group of Hanadi Sleiman, also at McGill, to develop protocols for the assembly of hybrid inorganic-DNA structures. He joined McMaster University in 2000, where he has established a research program that explores the use of heavy main-group elements in supramolecular systems and nonlinear optical materials. Regarding undergraduate education, he has lately been dedicated to the development of inquiry and integrated laboratory courses for chemistry majors. He is currently the Associate Chair for Undergraduate Studies in his Department.

Our Keynote Speakers



Born in Nova Scotia, Canada, Dr. Susan E. Burke obtained her Bachelor's Degree in Chemistry from St. Francis Xavier University where she worked on the investigation of the interactions of polymers and surfactants in solution as well as the physico-chemical properties of microemulsions; among other things. She then attended McGill University in Montreal, where she first obtained her Masters and then her PhD. Her work during her graduate career focused on the construction of polyelectrolyte multilayered films on planar surfaces and nanoparticles; as well as conducting kinetic and mechanistic studies on the morphological transitions in block copolymer aggregates. Her academic career led to numerous presentations as well as 21 peer-reviewed journal publications. In 2004 Dr. Burke started at Bausch & Lomb Inc. in Rochester, NY working in Global Research & Development where she now holds the title of Principle Scientist & Project Manager. She leads a technical team of formulation scientists focused on the innovation of new solution formulations for lens care. She is also the inventor and technical lead for the development of new contact lens care product (FDA approved) with projected annual revenues of >\$100 million. In her short time at Bausch & Lomb she already has 17 patents pending.

Oral Presentation Session #1

Room: St. Vincent Hall (301)

Moderator: Dr. Timothy Gregg
Niagara University

Abstract	Time	Speaker:
ORAL01	10:10 am	Kevin MacVittie , Guinevere Strack, Jian Zhou, Marcos Pita, Evgeny Katz <i>Clarkson University, NY</i> "Set-Reset Flip-Flop Memory Based on Enzyme Reactions: Toward Memory Systems Controlled by Biochemical Pathways"
ORAL02	10:35 am	Stacia Wegst , Jerry Tso, Rudolf Schneider, Diana Aga <i>University at Buffalo, SUNY</i> "Optimization of an Enzyme-linked Immuno-sorbent Assay and Sample Clean-up for the Analysis of 17 β -Estradiol in Poultry Litter"
ORAL03	11:00 am	Jared B. Wiseman , Nick Burke, Jafar Mazumder, Harald Stöver <i>McMaster University, Hamilton, ON, Canada</i> "Design of Polymers for Microencapsulation"
ORAL04	11:25 am	Paolo Gresta , Brittany Sumbler, Ronny Priefer <i>Niagara University, NY</i> "Comparison of Na(CN)BH ₃ and Si-CBH; Reductive Amination Agents"

Oral Presentation Session #2

Room: St. Vincent Hall (301)

Moderator: Dr. Christopher Stoj
Niagara University

ROOM 1

Abstract	Time	Speaker:
ORAL05	10:10 am	Justin Griffiths , Ronny Prierer <i>Niagara University, NY</i> "Iodinated Cubane Derivatives and their Thermal Properties"
ORAL06	10:35 am	Derek M. Peloquin , Philip Coppens <i>University at Buffalo, Buffalo NY</i> "A Theoretical Comparison to Observations on Bis(4-chlorothiophenol)(1,10-phenanthroline) zinc(II)"
ORAL07	11:00 am	Daniel G. Oblinsky , Stuart M. Rothstein <i>Brock University, St. Catharines, ON, Canada</i> "Reptation quantum Monte Carlo with application to the water molecule"

Poster Presentations (1:00-2:00)
St. Vincent Hall (4th floor)

- POST01 **Hannah Valdes, Mark Saric, Mary O'Sullivan**
 Canisius College, Buffalo, NY
 "Inhibition of *Trypanosoma cruzi* Trypanothione Reductase
 by Polyamines with Aromatic Substituents"
- POST02 **Russell C. Goodman, Theresa L. Beaty**
 Le Moyne College, Syracuse, NY
 "Prediction of Binding Sites on Nucleic Acid Binding
 Intrinsically Unstructured Proteins"
- POST03 Jan Duchek, Graeme Piercy, **David M. Ileski**, Tomáš Hudlický
 Brock University, St. Catharines, ON
 "Alternate Routes for the Synthesis of (+) – Codeine"
- POST04 **Hillary C. Chartrand, Kaitlin M. Smith, Karen E. Torraca**
 Houghton College, Houghton, NY
 "‘Green’ Oxidations of Alcohols Using Palladium-Catalyzed
 Reactions"
- POST05 **Robert V Dennis**, Kristen Baroudi, Vincent Lee, Sarbajit Banerjee
 University at Buffalo, Buffalo, NY
 "Synthesis, Fabrication, and Characterization of Conductive
 Graphene Films"
- POST06 **Jay J. Kim**, Matthew Frith, Janet R. Morrow
 University at Buffalo, Buffalo, NY
 "Selective Nucleotide Detection by a Eu(III) Phenanthroline
 Complex, Free and Incorporated into DNA"

- POST07 **Andrew M. Pinkham**, Thomas D. Kim
Rochester Institute of Technology, Rochester, NY
“Aminoguanidine down regulates expression of MreB RNA
in *Bacillus subtilis*”
- POST08 **AnneMarie Laurri**, Shella Dargout, Christopher S. Stoj
Niagara University, Niagara University, NY
“Expression, Purification, and Kinetic Characterization of
FET5 from *Saccharomyces cerevisiae*”
- POST09 **Brittany L. Sumbler**, Haley McClory, Lawrence Mielnicki, Mary McCourt
Niagara University, Niagara University, NY
“Development of an Early Detection Method For Alzheimer’s
Disease”
- POST10 **Haley McClory**, Lawrence Mielnicki, Mary McCourt
Niagara University, Niagara University, NY
“¹H NMR-Based Metabolomic Profiling of Patients with
Risk Factors of Coronary Artery Disease”
- POST11 **Charles Smith**, Haley McClory, Lawrence Mielnicki, Mary McCourt
Niagara University, Niagara University, NY
“The Synthetic Development and Structural Characterization
of Cholestosomes”
- POST12 **Shawn D. McGranaghan**, Sarah E. Morris, David G. Hilmey
St. Bonaventure University, Hamburg, NY
“Thinking locally in natural product isolation : The
purification and beginning analysis of *Sassafras albidum*
leaves and root inspired by Seneca Nation traditional
medicine”
- POST13 **William Femec**, Christopher Wirth, Lawrence Mielnicki, Mary McCourt
Niagara University, Niagara University, NY
“Molecular Model Building of CholestosomesTM and Anti-
Infective Analogs”

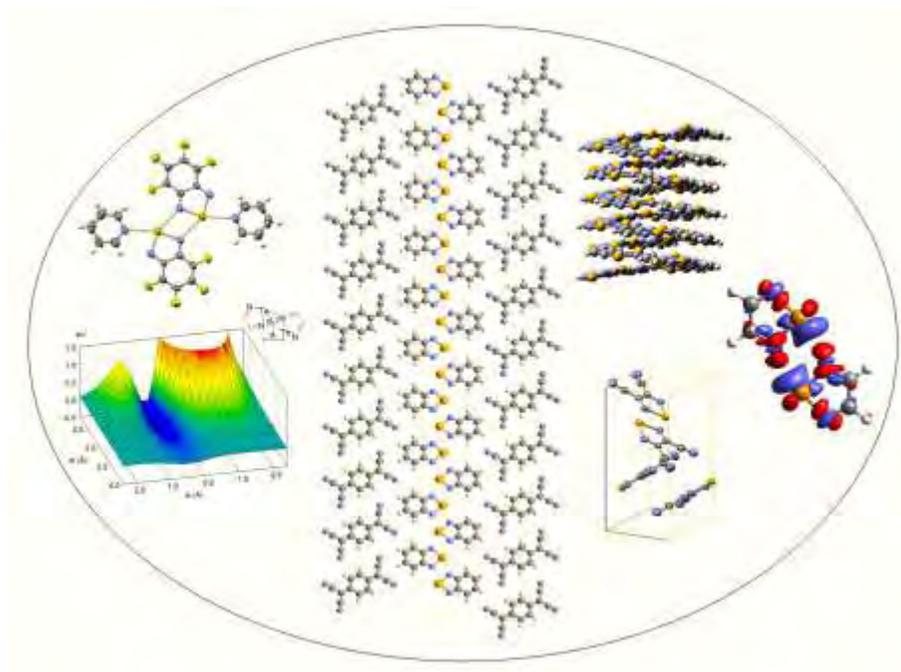
- POST14 **Nidya Dewi**, Jesus Velazquez, Javid Rzayev, Sarbajit Banerjee
University at Buffalo, Buffalo, NY
“Nanoporous Polypyrrole Membranes and Nanotube Arrays
from Fe₂O₃ Nanowire Array Templates”
- POST15 **Russell F. Algera, Furqan Hassan, Robert J. Stewart**, Timothy M. Gregg
Canisius College, Buffalo, NY
“Electronic control of intermolecular allene cyclopropanation
mediated by chiral dirhodium catalysts”
- POST16 **Alison W. Smith**, Pavel Belov, Ronny Priefer
Niagara University, Niagara University, NY
“Microwave-Assisted Methylation of Phenols with
DMF-DMA”
- POST17 **Michelle Emery**, Brian D. Leskiw, Josef G. Krause, Mary P. McCourt,
Ronny Priefer
Niagara University, Niagara University, NY
“Novel Approach in Synthesizing Substituted Hydroxyureas”
- POST18 **Kyle Biegasiewicz**, James Papia, Ronny Priefer
Niagara University, Niagara University, NY
“Novel Synthetic Route to a Library of Isoflavone
Derivatives”

Supramolecular Main-Group Chemistry: From Fundamental Bonding Studies to Functional Materials

Anthony F. Cozzolino, Phillip J.W. Elder, Lucia (M.) Lee, Qin Yang, Ignacio Vargas-Baca

Department of Chemistry and Chemical Biology, McMaster University, 1280 Main Street West,
Hamilton, Ontario, Canada L0R 1W0

In the crystal structures of their compounds, heavy main-group elements often display contacts with other atoms at distances significantly shorter than the sum of van der Waals radii but longer than the single hypervalent bond. Such Secondary Bonding Interactions (SBIs) are dative covalent bonds with small dissociation energies and thus have potential to drive the organization of supramolecular assemblies. However, the successful application of main-group SBIs depends on the identification of optimal *supramolecular synthons*. These are the structural elements that emerge due to operations of supramolecular synthesis. Molecules containing the 1,2,5-telluradiazole heterocycle are promising building blocks because of their propensity to create dimers or ribbon polymers through the formation of the $[\text{Te-N}]_2$ supramolecular synthon. This is a virtual four-membered ring containing two antiparallel Te-N SBIs and features good strength, directionality and reversibility. In early computational investigations, we examined details of the bonding and structure of such systems and showed that steric constraints as well as the attachment of Lewis acids or bases can control the degree of association of these molecules. Recently, we have applied telluradiazole heterocycles in the construction of three-dimensional lattices. The potentially useful properties of these materials will be illustrated through studies of thermochromism, solvatochromism, second harmonic generation and their self-assembly into molecular wires.



Chemistry of Vision Care Technologies

Susan E. Burke, Ph.D.

Lens Care Formulations Development Department, Vision Care R&D, Bausch & Lomb Inc.

Contact lenses have been used for vision correction since the first pair was developed in the late 19th century. The earliest versions of contact lenses were made from blown glass. However, over the years, the technology has evolved to encompass polymer based materials for improved patient tolerance and biocompatibility. In addition, contact lens care has also evolved for improved convenience and product performance. This presentation will focus on the advances in chemistry that have led to modern day contact lenses and lens care products.

Oral Presentation Abstracts

ORAL01

Set-Reset Flip-Flop Memory Based on Enzyme Reactions: Toward Memory Systems Controlled by Biochemical Pathways.

Kevin MacVittie, Guinevere Strack, Jian Zhou, Marcos Pita and Evgeny Katz

Department of Chemistry and Biomolecular Science, and NanoBio Laboratory (NABLAB), Clarkson University, Potsdam, New York 13699-5810

ABSTRACT: The enzyme-based set-reset flip-flop memory system was designed with the core part composed of horseradish peroxidase and diaphorase biocatalyzing oxidation and reduction of redox species (2,6-dichloroindophenol or ferrocyanide). The biocatalytic redox transformations were activated by H₂O₂ and NADH produced in situ by different enzymatic reactions allowing transformation of various biochemical signals (glucose, lactate, D-glucose-6-phosphate, ethanol) into reduced or oxidized states of the redox species. The current redox state of the system, controlled by the set and reset signals, was read out by optical and electrochemical means. The multi-well setup with the flip-flop units separately activated by various set/reset signals allowed encoding of complex information. For illustrative purposes, the words “Clarkson” and then “University” were encoded using ASCII character codes. The present flip-flop system will allow additional functions of enzyme-based biocomputing systems, thus enhancing the performance of multi-signal biosensors and actuators controlled by logically processed biochemical signals. The integrated enzyme logic systems and flip-flop memories associated with signal-responsive chemical actuators are envisaged as basic elements of future implantable biomedical devices controlled by immediate physiological conditions.

ORAL02

Optimization of an Enzyme-linked Immunosorbent Assay and Sample Clean-up for the Analysis of 17 β -Estradiol in Poultry Litter

Stacia Wegst¹, Jerry Tso¹, Rudolf Schneider², Diana Aga¹

¹Chemistry Department, University at Buffalo, Buffalo, NY, 14226

²BAM Federal Institute for Materials Research and Testing, Richard-Willstätter-Str. 11, 12489 Berlin, Germany

ABSTRACT: The occurrence of synthetic and natural hormones in the environment has recently raised great concern in both the scientific and mainstream media because of their endocrine disrupting properties even at very low (ng/L) levels. Quantification of hormones in environmental samples is very challenging because of their strong sorptive nature, requiring harsh conditions for extraction prior to sample analysis. In turn, the extracts typically contain high amounts of complex matrix that interferes with detection of hormones at very low levels. The use of enzyme-linked immunosorbent assay (ELISA) to determine estrogenic hormones provides an alternative tool for a cost-effective and fast screening of samples. However, matrix effects may still be encountered causing an unacceptable number of false positives. Therefore minor sample clean-up is still necessary to optimize the performance of ELISA. In this study, we optimized an accelerated solvent extraction, solid-phase extraction, and ELISA method for the trace analysis of 17 β -estradiol in poultry litter samples. This study aims to provide an effective screening tool that will be used in a large watershed-scale study on the fate and transport of 17 β -estradiol in croplands where raw and treated poultry litter has been applied.

ORAL03

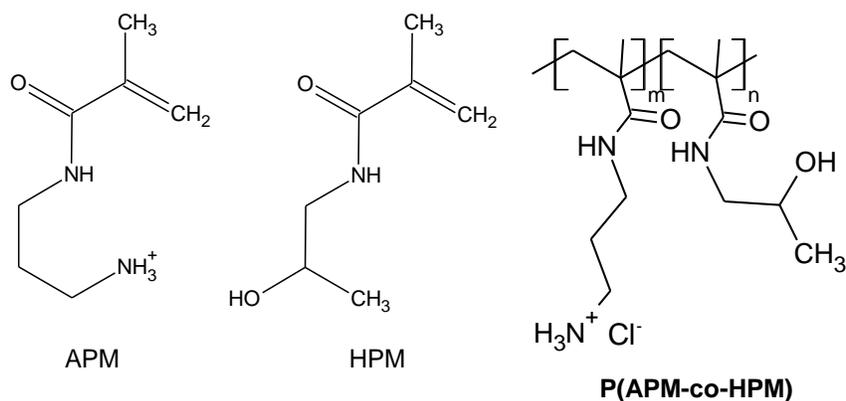
Design of Polymers for Microencapsulation

Jared B. Wiseman, Nick Burke, Jafar Mazumder, and Harald Stöver

Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON

ABSTRACT: Cell encapsulation is a promising method for the treatment of diseases such as diabetes, dwarfism, cancer, haemophilia, and lysosomal storage disorders. Charged polymers, or polyelectrolytes, are key components of the cell encapsulation system that are coated directly onto the cells or onto the surface of a hydrogel containing the cells. The polyelectrolyte coating isolates the **cells from the host's immune system, while allowing bidirectional diffusion of small molecules** such as nutrients, oxygen, and the therapeutic products formed by the encapsulated cells.

Microcapsules based on alginate are currently being used as the primary method for immunoisolation. These capsules have an alginate core coated with poly-L-lysine (PLL), and finally another layer of alginate. Problems that arise when using PLL and many other polycations, such as high costs, protein binding, and stimulation of the immune system, have led us to develop a new polycation layer to replace PLL, based on a copolymer formed from 3-aminopropyl methacrylamide (APM) and 2-hydroxypropyl methacrylamide (HPM). A series of copolymers with different charge densities (APM contents), including fluorescently labelled analogs, were prepared and characterized. Subsequently, the ability of these polycations to bind to alginate capsules and their distribution in the microcapsules were determined with techniques such as conventional and confocal microscopy.



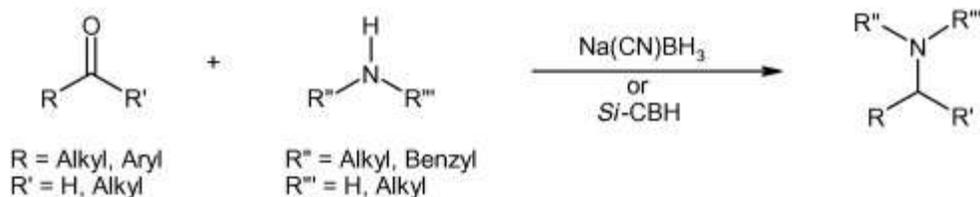
ORAL04

Comparison of $\text{Na}(\text{CN})\text{BH}_3$ and *Si*-CBH; Reductive Amination Agents

Paolo Grenga, Brittany Sumbler, Ronny Priefer

Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY 14109

ABSTRACT: Reductive amination is a chemical reaction commonly employed by organic chemists in academics and the pharmaceutical industry. In this reaction a carbonyl group is converted to an amine via an imine intermediate, the formation of which is rate limiting. A major reagent necessary for the completion of this reaction is a hydride source, commonly sodium cyanoborohydride ($\text{Na}(\text{CN})\text{BH}_3$). The objective of this research was to compare the efficacy of $\text{Na}(\text{CN})\text{BH}_3$ with silica-bound cyanoborohydride (*Si*-CBH) as hydride sources in reductive amination reactions. Work has shown that reactions employing *Si*-CBH as a hydride source showed significant improvement, exhibiting an average percent conversion 25% greater than reactions using $\text{Na}(\text{CN})\text{BH}_3$.



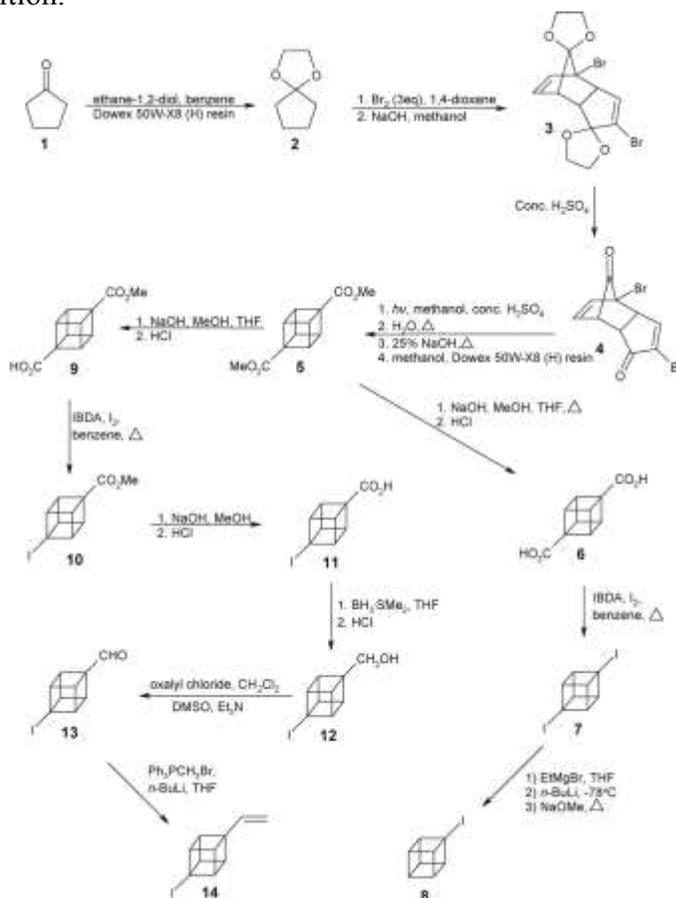
ORAL05

Iodinated Cubane Derivatives and their Thermal Properties

Justin Griffiths, Ronny Priefer

Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY 14109

ABSTRACT: Since the initial synthesis of cubane, numerous derivatives have been made with a diverse range of physical, chemical, and biological properties. Some iodinated cubane derivatives have been reported to be thermolytically unstable and/or rearrange in situ. An iodinated cubane-containing, norbornene-based polymer showed rapid thermo-decomposition during TGA studies. Bis-(4-iodocubylmethyl)-dialkoxy disulfide undergoes fragmentation more easily than its non-iodinated counterpart. The synthesis and thermal behaviour of a library of iodinated cubane compounds are herein reported. Most of the iodinated cubane derivatives showed melting/decomposition with no exotherm upon cooling. 4-Iodo-1-vinylcubane was observed to rearrange to 4-vinyl-trans- β -iodostyrene and its cyclooctatetraene intermediate during DSC analysis. TGA studies on 1-iodo-4-(hydroxymethyl)-cubane suggest that this particular iodinated cubane scaffold is mostly prone to rapid thermo-decomposition.



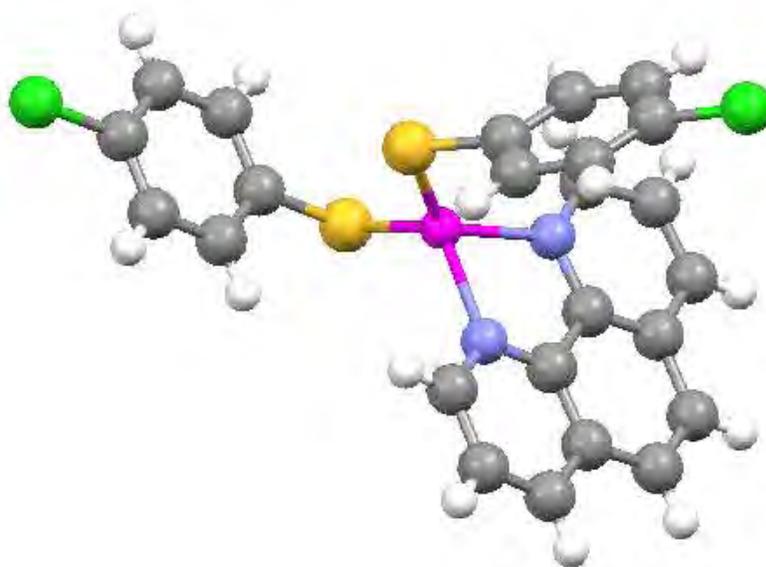
ORAL06

A Theoretical Comparison to Observations on Bis(4-chlorothiophenol)(1,10-phenanthroline)zinc(II)

Derek M. Peloquin, Philip Coppens

Chemistry Department, University at Buffalo, Buffalo NY 14260-3000

ABSTRACT: Bis(4-chlorothiophenol)(1,10-phenanthroline)zinc(II) is a compound which has two long lifetime emissions upon electronic excitation at low temperatures, indicating phosphorescence after singlet-triplet intersystem crossing. One of the emissions has been attributed to an interligand charge-transfer, the other to a π to π^* transition on the phenanthroline ligand, the relative intensities being a function of the temperature. The computer calculated spectra and orbitals of the singlet states confirm the existence of multiple bands, with transitions of electrons between the different ligands. The lowest triplet state, from which the emission is likely to occur, shows a significant shortening of the S-S distance, indicating the formation of a weak bond between these two atoms in the excited state. The geometry optimization of the isolated singlet state only approximately reproduces the values of the molecular geometry in the crystal. Two differently sized basis sets and the Gaussian program were used in the calculation to examine the dependence of the geometry on the computational details.



ORAL07

Reptation quantum Monte Carlo with application to the water molecule

Daniel G. Oblinsky, Stuart M. Rothstein

Department of Chemistry, Brock University, St. Catharines, ON

ABSTRACT: Reptation Quantum Monte Carlo (RQMC), first introduced by Baroni and Moroni has been applied to several important problems in physics, but with only a few applications to electronic structure problems.^{1,2} Through the use of a Markov chain and Metropolis-Hastings type algorithm one can both generate and sample the exact ground state electronic probability density. Different variants of the RQMC algorithm will be explored with the objective to increase both accuracy and precision of given observables. These include the dipole, quadrupole and octupole moments, parallel and anti-parallel electron interactions, and the energy.

¹ Baroni, S. and Moroni, S. *Phys. Rev. Lett.* **82** 4745 (1999)

² Yuen, W., Farrar, T., and Rothstein, S. *J. Phys. A: Math. Theor.* **40** F639 (2007)

Poster Abstracts

POST01

Inhibition of *Trypanosoma cruzi* Trypanothione Reductase by Polyamines with Aromatic Substituents

Hannah Valdes, Mark Saric, Mary O'Sullivan

Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY 14208

ABSTRACT: Certain members of the family Trypanosomatidae are protozoan parasites that cause human diseases including Chagas' disease in South America (*Trypanosoma cruzi*) and trypanosomiasis in Africa (*T. brucei* subspecies). Trypanosomatids have a unique antioxidant metabolism in which the enzyme, trypanothione reductase (TR), plays a central role. This enzyme catalyzes the NADPH reduction of a disulfide of trypanothione. Trypanothione is an unusual glutathione-spermidine conjugate (N^1, N^8 -bis(glutathionyl)spermidine) and the reduced (dithiol) form of trypanothione acts as a reducing agent in several vital processes including maintenance of the parasites' cellular thiol redox balance and reduction of tryparedoxin (which is a substrate for ribonucleotide reductase). Thus inhibitors of TR have potential as novel anti-trypanosomal chemotherapeutics. Here we report the syntheses of several novel polyamines, and studies of the inhibiting effects of these compounds on recombinant *T. cruzi* TR. The polyamines investigated were spermidine (*N*-(3-aminopropyl)-1,4-diaminobutane) and spermine (*N,N'*-bis(3-aminopropyl)-1,4-diaminobutane) derivatives with *N*-aromatic substituents.

POST02

Prediction of Binding Sites on Nucleic Acid Binding Intrinsically Unstructured Proteins

Russell C. Goodman, Theresa L. Beaty

Le Moyne College, Townhouses 203A, Syracuse, NY 13214

ABSTRACT: The method of analyzing intrinsically unstructured proteins (IUPs) to date has been limited to sequence analysis that attempts to predict intrinsically unstructured regions of proteins. However, our research is based on developing algorithms for predicting ligand binding sites and the associated secondary structure of these binding sites in IUPs. Our algorithms are founded on parameters determined through a statistical method, which used the Protein Data Bank, to calculate the frequency of all 20 amino acids occurring at the binding sites of 9 nucleic acid binding IUPs. Our primitive sequence composition algorithm for predicting binding sites, SeqCom, predicts, on average, 86.7% of the binding sites with 49.2% of the binding sites predicted representative of the native binding sites. To improve binding site prediction, we developed IUPattern. IUPattern works on the same principles as SeqCom, but it uses additional binding site constraints to better decipher between native and non-native binding sites. IUPattern predicts, on average, our 92.3% of the binding sites with 56.7% of the binding sites predicted representative of the native binding sites. In future work, we hope to incorporate binding site and secondary structure prediction into one algorithm. The predicted sequence will be annotated to show our confidence in the predictions.

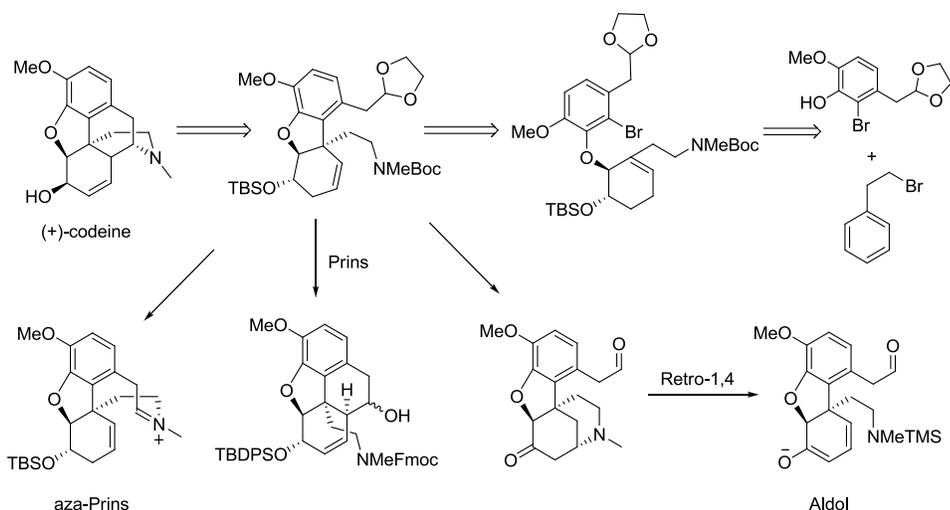
POST03

Alternate Routes for the Synthesis of (+) – Codeine

Jan Duchek, Graeme Piercy, David M. Ileski, Tomáš Hudlický

Brock University, Department of Chemistry, 500 Glenridge Avenue, St. Catharines, Ontario, Canada L2S 3A1

ABSTRACT: An interest developed for the synthesis of morphine alkaloids as a result of their potent biological activity and unique structure. Over the past fifty years, some thirty syntheses of morphine have been reported. Rice's synthesis in 1980 has proven to be the most efficient with a 29% overall yield. Therefore, the provision of morphine alkaloids by synthesis at a cost comparable to their isolation from natural sources remains a long-term goal of our research. The objective is to develop a route for an efficient and practical synthesis of *ent*-codeine from β -bromoethylbenzene using three routes from an advanced common intermediate. Current progress toward this goal will be reported.



POST04

“Green” Oxidations of Alcohols Using Palladium-Catalyzed Reactions

Hillary C. Chartrand, Kaitlin M. Smith, Karen E. Torraca

Houghton College, Houghton, New York 14744

ABSTRACT: In the field of organic chemistry much research has focused on the formation of carbon-carbon bonds for building complex molecules. One of the most commonly used methods for making carbon-carbon bonds is the aldol reaction which requires the use of aldehydes and ketones. Thus, the formation of this type of functional group is key to the synthesis of complex organic molecules. One of the standard reactions used to generate this functional group is the direct oxidation of alcohols to aldehydes or ketones. Although there are many current synthetic organic methods for completing this oxidation, many of them have the drawbacks of using stoichiometric amounts of heavy metals, hazardous reagents or solvent-intense extractive work-ups that make these reactions difficult to employ at large scale. In light of this, our research is focused on the development of a mild and green oxidation method that would be amenable to implementation at large scale where the greatest environmental impact could be made. Our initial efforts have focused on the use of palladium catalysis to complete this oxidation. Reagents we examined included various palladium sources, bases, solvents, and other additives. Although our best reaction conditions only produced on the order to 30% oxidized product, the reaction conditions were mild and required no harsh oxidants. Future research will focus on understanding the relationship between conversion and temperature as well as the nature of the palladium source.

POST05

Synthesis, Fabrication, and Characterization of Conductive Graphene Films

Robert V Dennis, Kristen Baroudi, Vincent Lee, Sarbajit Banerjee

Department of Chemistry, University at Buffalo, Buffalo, NY

ABSTRACT: Graphene, a single layer of graphite, is a highly conductive material with immense potential for use in the next generation of electronics applications. The potential for realizing ballistic conduction and its fascinating thermal and mechanical properties make graphene an interesting candidate in flexible electronics, conductive inks, ultracapacitors, and as fillers in polymers. Synthesis of graphene begins with the oxidation of graphite to graphite oxide and subsequent exfoliation to graphene oxide through ultrasonication. The graphene oxide can then be reduced to graphene using hydrazine or other reducing agents. We present here two distinctive methods for the fabrication of large-area conductive graphene films on conductive and non-conductive substrates. The first method involves the electrophoretic deposition of graphene oxide and reduced graphene oxide from aqueous solutions onto conductive substrates such as indium tin oxide and steel. The second method involves transfer printing of graphene oxide and reduced graphene oxide onto non-conductive substrates including glass and plastic. Characterization of the graphene films was carried out using near-edge X-ray absorption fine structure (NEXAFS), Raman spectroscopy, profilometry and four-point probe electrical conductivity measurements. NEXAFS was used to probe the electronic structure and alignment of these chemically modified graphene films. Raman spectroscopy and conductivity measurements were used to study the effect of reduction of graphene oxide to reduced graphene oxide.

POST06

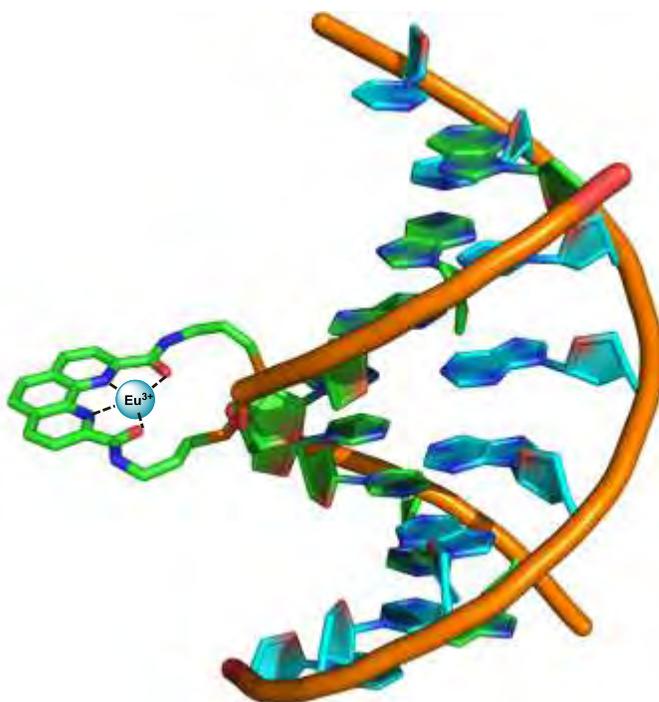
Selective Nucleotide Detection by a Eu(III) Phenanthroline Complex, Free and Incorporated into DNA

Jay J. Kim, Matthew Frith, Janet R. Morrow

Department of Chemistry, University at Buffalo, State University of New York, Amherst, NY

ABSTRACT: Lanthanide(III) complexes can be utilized as MRI contrast agents or optical sensors. These useful applications derive from the favorable luminescence and magnetic properties of Ln(III) complexes. Incorporation of the Ln(III) complex into DNA enhances recognition properties and facilitates the preparation of nucleic acid switches that respond to a particular anion. Here we show that one such phenanthroline-derived complex, PHEN-AE, binds Eu(III) both as a free ligand and as a non-nucleosidic linker incorporated into DNA. The Eu(III) complex of PHEN-AE was titrated with various nucleotides and analyzed by using direct excitation spectroscopy of the Eu(III) transition between 7F_0 to 5D_0 states with luminescence monitored at 618 nm. In the absence of nucleotides, Eu(III) retains 5 water molecules. In the presence of nucleotides including 5'-AMP, 3'AMP, 3'-CMP, 3'UMP, the Eu(III) loses at least one water ligand to give PHEN-AE Eu(III) nucleotide complexes with distinct dissociation constants. PHEN-AE, incorporated into DNA to give both single-stranded and bulge-like structures, binds Eu(III) up to 1000-fold more strongly than the free ligand.

Binding of 5'-AMP to the Eu(III)-DNA conjugate is sequence dependent.



POST07

Aminoguanidine down regulates expression of MreB RNA in *Bacillus subtilis*

Andrew M. Pinkham, Thomas D. Kim

Department of Chemistry, Rochester Institute of Technology, Rochester, NY

ABSTRACT: A significant link has been established between the regulation of iron homeostasis and a class of metalloenzymes known as multicopper oxidases. This research seeks to develop a deeper understanding of metallobiochemistry through the purification and characterization of the multicopper oxidase Fet5p from the baker's yeast *Saccharomyces cerevisiae*. Fet5p is directly involved in the oxidation of iron(II) and thereby the mobilization of iron stores from the yeast vacuole. *Pichia pastoris*, a strain of yeast which is notable for high protein expression as well as low glycosylation, was used as a proxy host in an effort to improve the expression of Fet5p. *FET5* was successfully cloned and integrated into the *Pichia* chromosome; however, attempts at isolation and purification of a functional Fet5p were unsuccessful. A new strategy has been implemented incorporating the plasma membrane ferroxidase Fet3p, a paralog to Fet5p, which has been truncated to secrete from the yeast cell. An expression vector containing an inactive form of *FET3* fused to *FET5* allowed for the successful secretion of functional Fet5p. Several separation techniques have been employed to purify the Fet5p including gel filtration and metal ion affinity chromatography. Additionally, further kinetic characterization of the intact chimera is underway.

POST08

Expression, Purification, and Kinetic Characterization of FET5 from *Saccharomyces cerevisiae*

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ABSTRACT: *Bacillus subtilis* has demonstrated the ability to synthesize the radical gas molecule nitric oxide (NO) through the activity of bacterial nitric oxide synthase (bNOS). However, our understanding of the role that NO plays in *B. subtilis* remains unclear. In this study we attempted to show that NO generated by bNOS regulates the cell wall synthesis protein mreB. Treatment of *B. subtilis* with aminoguanidine (AG), a known inhibitor of the structural homolog inducible NOS, has been shown to cause down-regulation of the mreB gene product. In this study, RT-PCR analysis of AG-treated *B. subtilis* demonstrates a down-regulation of mreB transcription. Also, treatment of cells with the antibiotic cefuroxime shows an increase in mreB expression. From these results, we can infer that NO plays a role in the regulation of cell wall biosynthesis and that this regulatory role may be involved in cell response to antibiotic stress.

POST09

Development of an Early Detection Method For Alzheimer's Disease

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ABSTRACT: Alzheimer's disease is a degenerative condition that affects over 5 million Americans with direct and indirect costs amounting to \$150 billion each year. It is the most common form of dementia resulting from the development of plaques and tangles in the brain that may block neuronal communication and lead to cell death and deterioration. This causes severe memory loss, confusion, difficulty with everyday tasks, and personality changes. There is currently no cure for Alzheimer's disease, so early detection is the key to saving lives. This research project aims to develop an early detection method for Alzheimer's disease by examining human urine samples using H^1 -NMR spectroscopy. The concentration of various metabolites found in the urine that are related to Alzheimer's disease will be quantified using the Chenomx-NMR Suite Version 6.0, and then the data will be analyzed using Umetrics SIMCA-P+ multivariate analysis software. The results of the data analysis will be correlated with the results of memory tests performed on the urine donors. The ultimate goal of this project is to develop a simple, noninvasive test that will be able to place individuals into groups depending on the level of development of the disease. Currently, Alzheimer's disease is diagnosed in its later stages when treatment options are limited; however, this project's ultimate benefit will be its ability to detect the disease in its earliest stages when the usual memory symptoms aren't yet noticeable.

POST10

¹H NMR-Based Metabolomic Profiling of Patients with Risk Factors of Coronary Artery Disease

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ABSTRACT: The prevalence of Coronary Artery Disease (CAD) in current well-developed countries has caused an increase in the amount and type of technology used to diagnose and treat this sometimes-debilitating disease. These techniques, which usually consist of invasive and sometimes painful procedures, have lead us to consider metabonomics as a way of determining CAD. Metabonomics is the study of the different metabolites and their concentrations in the body and is specific to the cellular processes that are carried out throughout the body.

In recent years there has been an increased desire to understand the usefulness of metabonomics using bio-fluids to determine various different processes that occur in the human body. Due to the wide variety and numbers of metabolites or biomarkers found in the metabolome the study of metabonomics had proved to be complex but effective. By using blood plasma from patients at risk for CAD and using proton NMR we are determining the metabolites associated with CAD.

POST11

The Synthetic Development and Structural Characterization of Cholestosomes

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ABSTRACT: Cholestosomes™ are novel nanoscale drug delivery vesicles synthesized from neutral lipids based on their co-solubility as determined from DSC measurements. Initial synthesis using cholesteryl Myristate and cholesteryl Laurate in a 1:1 molar ratio resulted in a vesicle, which incorporated a fluochrome (FITC) and was shown to be capable of drug delivery into cells. This study reports on a new synthetic procedure that increases productivity as well as extractive productivity. Electron Microcopy gives evidence of the nanoscale size as well as indication of the shape of the vesicles. Dynamic Light Scattering was also used to determine the size range of the vesicles. The most recent work includes successful incorporation of different chromophores as well as using different esters in different molar combinations in addition to the incorporation of oxysterols as a method for changing surface electrostatics. Surface properties are critical for the targeted delivery and survival in the body. Recent work also includes the development of an effective long-term storage procedure.

POST12

Thinking locally in natural product isolation : The purification and beginning analysis of *Sassafras albidum* leaves and root inspired by Seneca Nation traditional medicine

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Abstract: A natural product is a chemical or substance produced by a living organism that often has pharmacological or biological activity. The sassafras tree is a source of natural products that has been used by the Seneca Nation of Indians for many years for a variety of traditional remedies. For example, the Seneca Nation has used the leaves of sassafras as an anti-septic on wounds. There have been several studies illustrating compounds isolated from the leaves, bark, and roots of the sassafras tree by steam distillation. The focus of this project is to isolate compounds, determine structure, and run trials to test for anti-bacterial activity. In its beginning stages we have developed procedures for root and leaf extraction, performed TLC analysis of the mixtures, and isolated its known main component, safrole as a proof of principle.

POST13

Molecular Model Building of CholestosomesTM and Anti-Infective Analogs

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Abstract: Polymer surface coatings on liposomes enhance the directional delivery capabilities of the vesicle and in fact they can be considered to be stealth vesicles for targeted drug delivery. Several common polymer surface coatings that are used include polyethylene glycol (PEG), polyamines and poloxamers. These polymer surface coatings result in an electrostatic external surface which facilitates deliverability and availability in the body. Cholestosomes (TM), a recently developed nanoscale drug delivery system, has been shown to be able to deliver drugs to cells without the benefit of surface coatings. This study explores the electrostatic properties of the cholestosomes and analogs of drugs that could be potentially used with them. It will help determine whether the use of cholestosomes will expand the use of the given drugs. Analogs are built using SYBYL and then charges are calculated using the Tripos MM force field. Isopotential surfaces are then explored and compared to those of the cholestosomes. Cholestosomes are composed of neutral lipids that pack reflective of their crystallographic structures. Preliminary studies suggest an electrostatic compatibility between the cholestosomes and drug analogs.

POST14

Nanoporous Polypyrrole Membranes and Nanotube Arrays from Fe₂O₃ Nanowire Array Templates

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Abstract: Nanostructured conducting polymers are of interest for various technological applications including large-area solar panels, ultrafiltration, light-emitting displays, and optical/electrical sensors. In particular there is considerable interest in the fabrication and assembly of nanostructures and nanostructured membranes of conjugated polymers such as polypyrrole (PPy), polythiophene, and polyaniline that in the bulk form are known to be robust workhorses for a myriad of applications ranging from hybrid photovoltaics to flexible displays. Herein, we report the fabrication of PPy nanotube arrays and nanoporous membranes by electrophoretic deposition of pyrrole monomers onto Fe₂O₃ nanowire-array templates. A facile bottom-up process starting from carbonized steel has been developed to first obtain highly oriented Fe₂O₃ nanowire arrays, which subsequently serve as sacrificial templates for the electropolymerization of polypyrrole from aqueous solutions of pyrrole monomers. Systematic variation of electrodeposition and etching conditions enables control over the nanostructured morphology. The morphology, bonding and electronic structure of the as-deposited nanostructured PPy films have been characterized by scanning electron microscopy, near edge X-ray absorption fine structure (NEXAFS) spectroscopy, Fourier transform infrared spectroscopy, and Raman Spectroscopy.

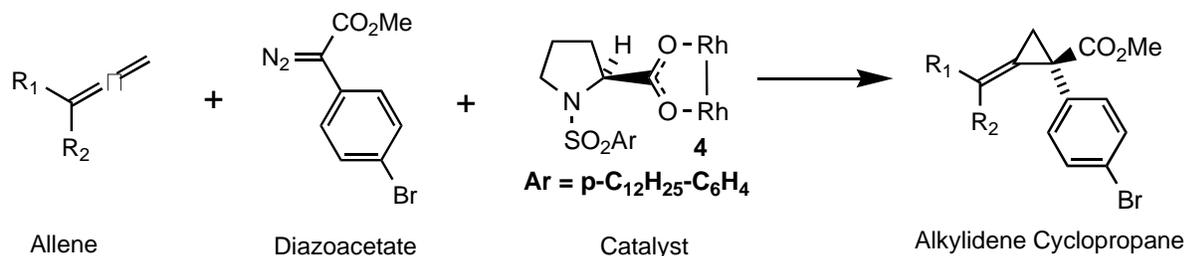
POST15

Electronic control of intermolecular allene cyclopropanation mediated by chiral dirhodium catalysts

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Abstract: Intermolecular cyclopropanation of monosubstituted allenes is a powerful method for preparing chiral alkylidene cyclopropanes. This efficient rhodium-catalyzed reaction can be subject to variability in the yield and enantioselectivity of products. Electronic effects of substituents can accelerate or retard the reaction rate. To improve the usefulness of the reaction, we are investigating electronic effects of aryl, alkyl, and silyl substitution on the rate of allene cyclopropanation. Our research involved cyclopropanation of a series of para-substituted phenylallene substrates in competition with the unsubstituted analog, indicating that reaction rates correlate with Hammett substituent coefficients. This is consistent with a mechanism involving buildup of positive charge at the central carbon of the allene substrate. We are also presenting the results of similar competition experiments, in which it was observed that alkyl substituents slow reaction rates, but that this steric effect can be offset in certain cases by β -silicon electronic effects, aiding the development of enantiomerically enriched alkylidene cyclopropanes for use in the synthesis of complex targets.



Favored product when R1 is larger than R2 or when R1=Si(CH₃)₃

POST16

Microwave-Assisted Methylation of Phenols with DMF-DMA

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Abstract: The methylation of phenol compounds is commonly performed in order to preserve the alcohol group(s) from interfering with subsequent reactions. This protection can be done in numerous manners, one of which is the use of *N,N*-dimethylformamide dimethylacetal (DMF-DMA). This however typically requires lengthy reflux (i.e. 24hrs). This project examines the use of microwave to accelerate the rate of reaction. This new process methylates in thirty minutes to one hour using a laboratory microwave and is dependent upon the electron donating and withdrawing substituents attached to the ring.

POST17

Novel Approach in Synthesizing Substituted Hydroxyureas

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Abstract: Hydroxyureas have been identified as an antiviral treatment for a number of diseases. A known technique for the synthesis of substituted hydroxyureas involves reacting hydroxylamines with potassium cyanate. The aim of this research was to provide evidence of our novel approach in creating these biologically active molecules. We were successfully able to synthesize a library of hydroxyureas by reacting a variety of amines with tert-butylmesitylenesulfonyloxycarbamate followed by deprotection.

POST18

Novel Synthetic Route to a Library of Isoflavone Derivatives

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Abstract: Isoflavones are a class of organic compounds that are almost exclusively found in members of the bean family including soybeans, chick peas, alfalfa, and peanuts. Their unique structure, composed of a three ring back bone including two aryl moieties, has been recognized for its beneficial antioxidant traits as well as its recognizable activity against certain types of cancer. They have most recently been recognized for their inhibitory activity against breast and colon cancer. This project is based on a novel three or four step synthesis of a library of isoflavone derivatives including ones such as Daidzein, an isoflavone and well known antioxidant found commonly in soybeans. The synthesis involves an enamine addition, a ring closure and iodination, and Suzuki coupling utilizing PEG10000 for a green approach to the reaction. This synthesis provides evidence of an efficient pathway to the synthesis of future isoflavones of interest.

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