The 2025

Undergraduate Research Symposium

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

Saturday April 5, 2025

Canisius University
BUFFALO, NY

Welcome Message from the Organizing Committee

Welcome to the 2025 Western New York American Chemical Society Undergraduate Research Symposium. Canisius University Department of Chemistry and Biochemistry and the Canisius Student ACS Club are pleased to host this year's event, highlighting the exciting research executed by the undergraduate students and their mentors from Western New York and surrounding areas.

Undergraduate research is often cited as the critical activity that inspired the professional careers of academic and industrial chemists, health professionals, and government scientists. Since its inception in Western New York in 2008, this American Chemical Society Undergraduate Research Symposium has brought together undergraduate researchers and their mentors from area colleges and universities to share their rich and diverse undergraduate research experience.

We thank our Keynote speaker, Dave Moz, of Syracuse University, for his participation in this event. In addition, I want to thank the members of the Organizing Committee of this symposium, the WNYACS Section, and Canisius University, all of whose efforts have made this event possible.

Sincerely,

Tim Gregg, Ph.D.
Chair, 2025 Symposium Committee

2025 Symposium Organizing Committee

Chair: Dr. Timothy M. Gregg
Dr. Corey Damon
Department of Chemistry and Biochemistry, Canisius University

Dr. Sherry Chemler
Department of Chemistry, University at Buffalo, SUNY

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The 2025 Western New York ACS Undergraduate Research Symposium

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Chemistry and Biochemistry
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ACS of Western New York

Schedule of Events

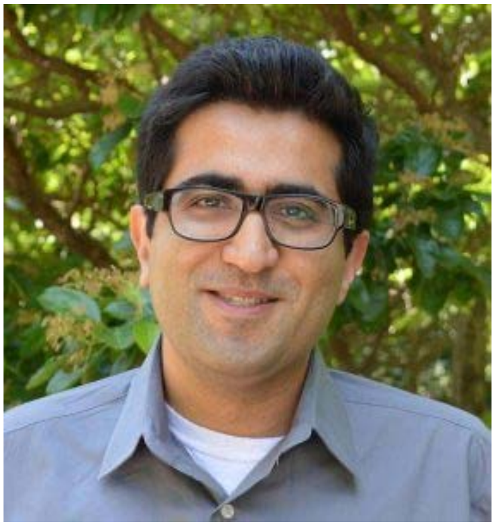
April 5, 2025

Canisius University

Winter Student Center

8:00 am – 8:50 am	Registration	(Student Center 2nd floor)
8:50 am – 9:00 am	Introductory Remarks	(Student Center Regis Room)
9:00 am – 10:00 am	Keynote Address: **Dr. Davoud Mozhdehi** Department of Chemistry, Syracuse University **Greasing the Protein Gears: Harnessing Lipidation for Next-Generation Biomaterials and Therapeutics**	
10:00 am – 12:00 pm	Student Oral Presentations	
12:00 pm – 1:30 pm	Lunch	
12:00 pm – 1:30 pm	Mad Scientist Photo Booth	(Student Center Regis Room)
1:30 pm – 3:00 pm	Student Poster Session	(Student Center Grupp Lounge)
3:00 pm	Symposium Awards and Closing remarks	(Student Center Regis Room)

Keynote Speaker



Davoud Mozhdehi (Dave Moz) is an Associate Professor of Chemistry at Syracuse University, where his research group focuses on bioinspired materials design. His NIH- and NSF-supported investigations center on harnessing post-translational modifications—such as lipidation—to develop smart biomaterials for applications in nanomedicine and biotechnology.

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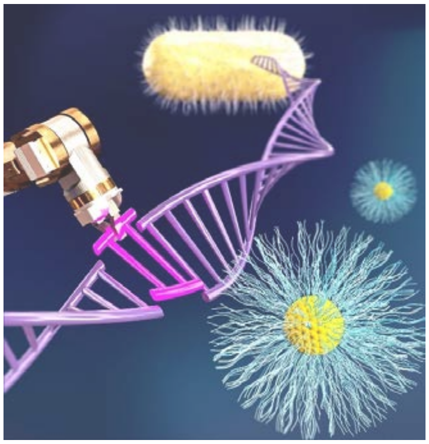
ROYAL SOCIETY OF CHEMISTRY

COMMUNICATION
Davoud Mozhdehi *et al.*
Non-canonical lipoproteins with programmable assembly and architecture

Davoud Mozhdehi
Syracuse University

Greasing the Protein Gears: Harnessing Lipidation for Next-Generation Biomaterials and Therapeutics



Abstract: Recent advances in recombinant DNA technology have enabled the precise design and production of protein-based materials, offering unprecedented control over their composition, structure, and function. Yet, the limited repertoire of canonical amino acids restricts the chemical diversity—and thus the functionality—of these biomaterials. To address this limitation, we draw inspiration from a solution offered by Nature: leveraging specific chemical transformations to modify proteins with non-proteinogenic building blocks, a process called post-translational modification (PTM), which expands the chemical diversity of the proteome by more than two orders of magnitude.

Motivated by this bioinspired strategy, my lab focuses on leveraging protein lipidation to create de novo hybrid biopolymers with programmable structure and function. Although the chemical biology of lipidation has garnered intense interest, methods for producing lipidated proteins in a scalable, cost-effective manner remain scarce. Conventional approaches are hindered by the ribosome's strict preference for amino acid-derived motifs or by labor-intensive and technically challenging semi-synthetic routes.

To overcome these hurdles, we have developed high-yield biosynthetic methods for producing lipidated proteins, enabling systematic investigation of their structure and properties. Our findings reveal that the nano-assembly and liquid–liquid phase separation behaviors of lipidated proteins diverge markedly from predictions based on synthetic polymeric surfactants or peptide–amphiphiles. Although lipid moieties represent only a small fraction of the overall molecular mass, their pronounced hydrophobicity significantly alters protein hydration and inter-domain interactions, exerting effects that extend well beyond the site of modification. Understanding this "molecular syntax" will pave the way to next-generation biomaterials and therapeutics capable of mirroring the sophisticated hierarchy and functionality observed in living systems.

Oral Presentations

9:00 AM - 12:00 PM Student Center Regis Room

9:00 am **Prof. Davoud Mohzdehi** Syracuse University

Keynote Address

Greasing the Protein Gears: Harnessing Lipidation for Next-Generation Biomaterials and Therapeutics

10:00 AM **Abe Ellenbogen** University of Rochester

Development of a New Method for N-Heterocyclic Carbene Functionalization

10:20 AM **Owen Szeglowski** University at Buffalo

Synthesis of Heterobimetallic Porphyrin Tubes for Modulation of Small Molecule Catalysis and Host-Guest Chemistry

10:40 AM **Adrian Martinez** Niagara University

Studies Toward the Synthesis of *ent*-Artemisinin, a Potential Anti-malarial Compound

11:00 AM **Rebecca Reagan** University of Rochester

Development of a Pyridonate-Ligand-Enabled Copper-Catalyzed Reaction

11:20 AM **Rakshith Sreeram** Cornell University

Generalizing Colloidal Synthesis for Non-Precious Metal Oxide Electrocatalysts

11:40 AM **Robert Suber** University at Buffalo

Redox-responsive Iron MRI Contrast Agents

Student Talk (1)

Development of a New Method for N-Heterocyclic Carbene Functionalization

***A. Benjamin Ellenbogen**, M. Afandiyeva, C. Rose Kennedy**

Department of Chemistry, University of Rochester, Rochester, NY

N-Heterocyclic Carbene (NHC) ligands bound to metal centers have significant catalytic applications due to their structural modularity coupled with strong sigma donating character. Over the past decade, symmetric aryl-substituted NHCs have been utilized in nickel-catalyzed cross-coupling reactions. These studies have elucidated the importance of aryl substitution patterns on reactivity at the metal center. In addition, there are preliminary studies with unsymmetric aryl NHCs suggesting greater tunability and control of the reaction pathways. However, these unsymmetric aryl-NHCs are underexplored due to the lack of robust synthetic routes to ligand synthesis. To overcome this challenge, my work has been focused on the functionalization of nickel-bound NHC ligands via in situ cross-coupling with bench-stable and easily accessible aryl boronic acid nucleophiles. This presentation will focus on the discovery and optimization of the nickel-mediated arylation in the 2 and 6 position of the aryl moieties on unsymmetric NHC ligands using a model system (Figure 1). My studies, supported by LC-MS and ^{1}H NMR, have shown the formation of mono- and di-substituted aryl-NHCs. Future studies will be conducted to appreciate the utility of this methodology for late-stage ligand diversification for transition metal catalysis.

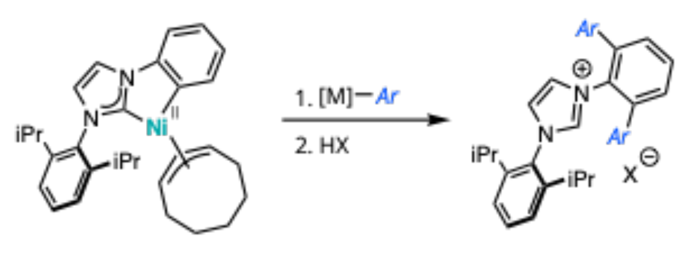


Figure 1. *[(hIPrPh)Ni(η^3-C_8H_{13})] was used as the model system for reaction discovery and optimization.*

Student Talk (2)

Synthesis of Heterobimetallic Porphyrin Tubes for Modulation of Small Molecule Catalysis and Host-Guest Chemistry

***Owen Szeglowski**, John Pinti, Matthew Crawley, and Timothy Cook**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Motivated by the ever-increasing demand for energy, the Cook lab has been continually exploring the use of polynuclear porphyrin architectures as catalysts for small molecule activation. Historically, metallic molecular clips have been employed to facilitate the assembly of these prisms, however it is attractive to eliminate these structural metals, as they are associated with higher costs and reduced acid stability. Herein, we report the synthesis and characterization of a tetra-porphyrin tube bridged by organic pyridinium-based linkers (Figure 1). These tubes can be post-synthetically metalated with a series of first-row transition metals, including Zn, Ni, and Co. Uniquely, as these tubes are the result of two distinct porphyrin moieties, they provide an ideal candidate for a heterobimetallic system, such as Zn$_2$-Co$_2$-tube. By controlling the metal sites present in this architecture, we can modulate the activity of the porphyrin tubes for catalysis of the oxygen-reduction reaction (ORR), in which the Co$_4$-tube has the lowest overpotential, followed by the Zn$_2$-Co$_2$-tube, and finally the Zn$_4$-tube. Beyond this, the size of the architecture makes them an ideal candidate for host-guest chemistry. To probe this, encapsulation of C$_{60}$ and C$_{70}$ were studied via absorbance and fluorescence routes, where the structures were found to asymmetrically accommodate the fullerenes, breaking the internal symmetry of the molecule and thus splitting the proton resonances further when encapsulated.

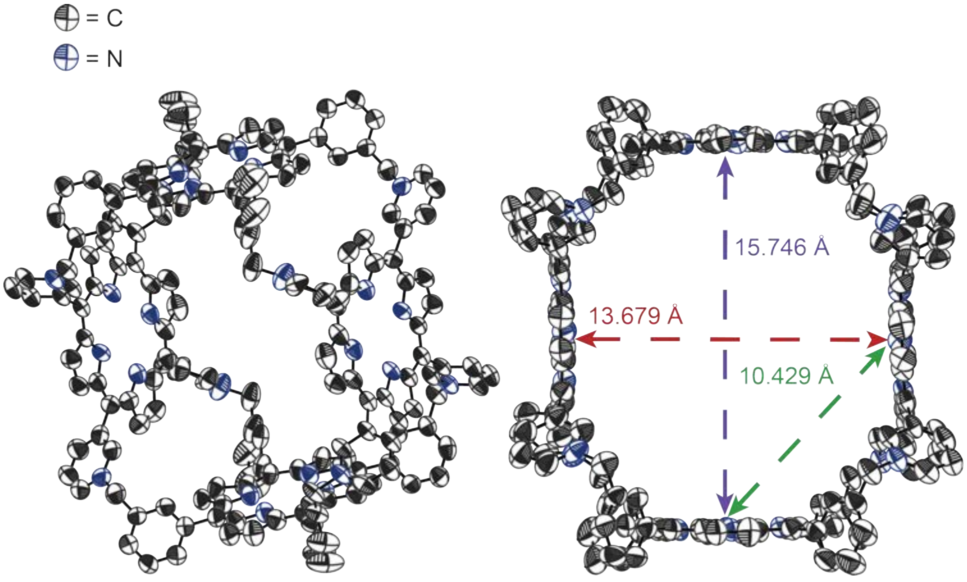


Figure 1: Ellipsoid crystal structure of FB4-tube. Hydrogen atoms, outer-sphere PF$_6^-$ ions, and co-crystallized DMF were omitted for clarity.

Student Talk (3)

Studies Toward the Synthesis of *ent*-Artemisinin, a Potential Anti-malarial Compound

***Adrian Martinez**, Emily Steiner, and Luis Sanchez**

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

Artemisinin is a natural product isolated from the plant *Artemisia annua* that is currently the fastest- acting treatment available against *Plasmodium falciparum*—the protozoan parasite that causes the deadliest form of malaria. The low bioavailability of this compound and its short half-life, however, make the cost of artemisinin therapies very high. Anti-malarial combination therapies involving artemisinin are employed to avoid the development of resistance to the drug by the parasite, as recommended by the World Health Organization.

Artemisinin's structure contains a unique peroxide bridge that is believed to be responsible for the drug's mechanism of action. Recent reports show that artemisinin binds covalently to a large number of proteins after being "activated" most likely by heme, which builds up in the parasite cells given its 'blood-eating' nature. The exceptional biological activity of this compound appears to originate in the fine-tuned chemical reactivity of its peroxide bridge, rather than the topology of the structure itself. It is expected that its enantiomer (*ent*- artemisinin) would be a viable alternative as an anti-malarial agent, if an affordable synthetic route were developed. The current goal of this project is to develop a reaction sequence to produce *ent*-artemisinin from zingiberene, a compound found in ginger oil. If successful, we believe that the low cost and high availability of ginger oil would allow for the large-scale production of *ent*-artemisinin.

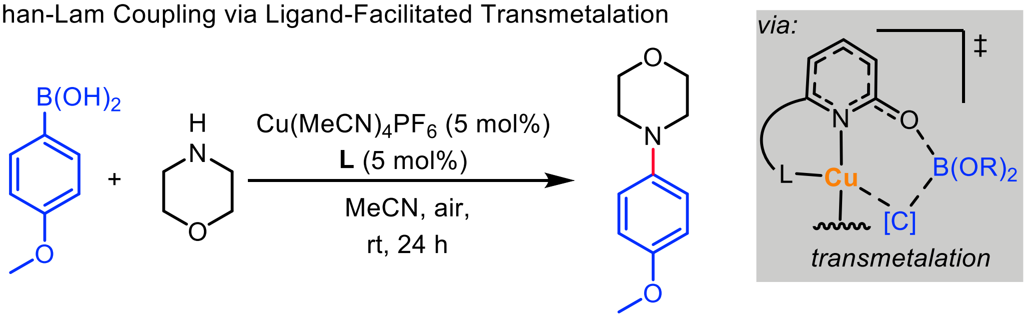
Student Talk (4)

Development of a Pyridonate-Ligand-Enabled Copper-Catalyzed Reaction

Rebecca S. Reagan*, Hailemariam Mitiku, C. Rose. Kennedy**

Department of Chemistry, University of Rochester, Rochester, NY

Chan-Evans-Lam Coupling generally involves the use of a Cu(II) salt to catalytically form C-N bonds using a cross-nucleophile coupling reaction. These C-N bonds are critical for pharmaceutical, agrochemical, and materials synthesis. The developed reactions are mechanistically understudied because of the difficulty in probing a salt-catalyzed reaction. Mechanistic ambiguity has necessitated the development of unique reaction conditions—copper source, base, water equivalents—to achieve successful coupling of different substrates. Despite this lack of a mechanistic consensus, it is proposed that the transmetalation from the boron nucleophile to the metal center is the first step of the catalytic cycle. We hypothesized that a pyridonate ligand could promote transmetalation of the boron nucleophile to copper center while simultaneously providing insight in the design of future C-N coupling reactions. We identified that the pyrazole-pyridonate (PzPyO) ligand enabled yields greater than 60%. In contrast, the yields of the unsubstituted derivative, methoxy derivative, 4-hydroxy derivative, and [Cu(MeCN)4]PF6 salt did not demonstrate comparable reactivity with the PzPyO ligand, suggesting that the 2-pyridone moiety plays a critical role in catalysis. With these results, we sought to characterize the copper species using SC-XRD and NMR and aim to optimize the yield of the reaction before progressing to mechanistic study of the reaction. These future directions will enable us to evaluate the structure-function relationship of the 2-pyridone ligand motif while simultaneously providing insight into Chan-Evans-Lam type coupling to access expanded substrate scope.


Chan-Lam Coupling via Ligand-Facilitated Transmetalation

Student Talk (5)

Generalizing Colloidal Synthesis for Non-Precious Metal Oxide Electrocatalysts

Rakshith Sreeram*, Xin Wang, Olivia Wong, Ryan Tse, and Héctor D. Abruña****

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY

Platinum-based electrocatalysts are widely employed in fuel cell applications such as transportation, energy storage, and conversion due to their exceptional catalytic efficiency and durability. However, their scarcity and high cost have precluded their widespread commercial adoption, driving the search for alternative, abundant, and economically viable electrocatalysts. Given that no single non-precious metal fully replicates the performance of platinum-based systems, incorporating multiple non-precious (typically first row) transition metals represents a promising alternative. Leveraging synergistic interactions among multiple cations allows precise tuning of electronic structures, lattice strain, and active site distribution, thus enhancing specific steps within electrocatalytic reactions. Building upon the promising catalytic activities demonstrated by cobalt-manganese spinel oxides, this work aims to synthesize metal oxides combining cobalt-manganese with an additional non-precious transition metal to further tune and improve their electrocatalytic performance and long-term durability.

Colloidal synthesis was systematically investigated under diverse reaction conditions, including variations in synthesis routes, temperatures, ligand selections, and metal precursors, so as to elucidate/establish correlations between synthesis parameters and performance. Comprehensive characterization via X-ray diffraction, scanning electron microscopy, and rotating disk electrode voltammetry experiments provided insights into crystallographic structures, elemental distributions, and electrocatalytic efficiencies of the synthesized oxides. Future integration of these findings into machine learning models will facilitate rapid identification of optimal synthesis conditions, significantly accelerating catalyst development. This research represents an important step toward sustainable, cost-effective electrocatalytic materials suitable for commercial-scale fuel cell and electrolyzer applications.

Student Talk (6)

Redox-responsive Iron MRI Contrast Agents

***Robert H. Suber**, Deepak Krishnan Balaji, and Janet R. Morrow**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Magnetic resonance imaging (MRI) contrast agents contain paramagnetic centers that generate a fluctuating magnetic field to decrease the longitudinal relaxation time (T_1) of *in vivo* water protons. Redox-responsive contrast agents are altered by biological environment, including tumor microenvironments, to affect the probe's relaxivity. Coordination complexes containing Fe(III) are promising alternatives to Gd(III) MRI contrast agents for the improved diagnostic accuracy of tumor detection and imaging. Complexes which register redox environment by switching between Fe(II) and high-spin Fe(III) with a redox potential of 200-400 mV are optimal. Redox potentials are tuned by ligand design. The macrocyclic ligand, 1,4,7-triazacyclonane (TACN), forms kinetically inert Fe(II)/Fe(III) complexes. Hexadentate ligands are comprised of TACN and pendant groups; hydroxypropyl pendants with TACN have been previously reported in the formation of high-spin Fe(III) complexes which are stable at neutral pH. This study employed pyridine and hydroxy propyl pendants for ligand synthesis to tune the redox potential of the iron center. The Fe(II) and Fe(III) complexes were characterized, towards their application as T_1-relaxivity, redox-responsive contrast agents.

Student Poster Presentations List

1:30 PM - 3:00 PM

Poster #

1. ***Olivia Wong**, Xin Wang, Rak Sreeram, Ryan Tse, and Héctor Abruña**

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY

Colloidal Synthesis Dataset Development of Non-Precious Metal Oxide Electrocatalysts for Oxygen Reduction Reaction

2. ***Grace E. Baumgartner** and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Computational Chemistry Study of Alkaline-Earth Monoamide Isomers

3. ***Brooke R. Stanley**, Shannon O'Neil, Owen E. Monteferrante, and Shauna M. Paradine**

Department of Chemistry, University of Rochester, Rochester, NY

Olefin Heteroannulation with Non-Aromatic Ambiphiles via Urea-Enabled Palladium Catalysis

4. ***Jenna L. Davies,**[1] ***Isabelle R. Prentice,**[1] *Michael D. Clark,*[2] *Zachery A. Schmidt,*[2] *Gregory J. Lapp,*[1] *Hannah R. Dierolf,*[1] *Kacie R. Liwosz*,*[1] *and David F. Watson*[2]

[1]Department of Natural Science and Mathematics, D'Youville University,
[2]Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Optimization of Dye-$CuAlO_2$ Films for Hydrogen Generation

5. ***Elise Spence**, Steele Burgeson, and Luis Sanchez**

Department of Biochemistry, Chemistry, and Physics, Niagara University

Development of a Biaryl Oxidative Coupling-Based Route to the Anti-Tumor Natural Products TMC-95

6. ***Aaron J. Szczepankiewicz, Emily R. Barry**, and Steven H. Szczepankiewicz**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Reduced Polytungstates in Nonpolar Environments

7. ***Zachary C. Ellis****, Gabrielle Shin, Alexander Ruhren, and Claire Besson**

Department of Chemistry, Binghamton University, Binghamton, NY

Synthesis and characterization of [Fe^{II}(4-BrTp)] for use in Spin-Crossover-Based Electronic Devices

8. ***Matthew T. Gleason****, Kaycie Malyk, Vivek G. Pillai, and C. Rose Kennedy**

Department of Chemistry, University of Rochester, Rochester, NY

Mechanistic Insight into Nickel-catalyzed Conjunctive Cross-coupling of Amides

9. ***Jacob P. Smeraldo*** *and Alexander J. Rupprecht**

Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY

Self-Assembled Monolayers: A Transition from Disordered to Ordered, and Their Applications in the Industrial and Biomedical Fields

10. ***Zachary E. Holmes***[1]*, Matthew R. Crawley*[2]*, and Lauren E. Rosch**[1,2]

[1]Department of Biochemistry, Chemistry, and Physics, Niagara University
[2]Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Discovering Tellurium's Reactivity: Synthetic Progress Towards a Novel Benzo-fused Telluropyrylium Chromophore

11. ***Alex B. Szczepankiewicz*** *and Corey Damon**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Haloperoxidase Biomimicry: Toward the Generation of Electrophilic Species Utilizing Xerogel-Based Transition Metal Catalysts

12. ***Dhani V. Slaughter****, Noelle M. Linenfelser, and Karen E. Torraca**

Department of Chemistry, Houghton University, Houghton, NY

Green Anaerobic Oxidation of Alcohols

13. ***Amelia Kelly**, Stefano Racioppi, and Eva Zurek**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Computational Investigation into Aluminum Oxide (Al_2O_3) at Planetary Conditions

14. ***Reginald A. Annor**[1], Samson B. Zacate[1], Jonas Rein[1], Soren D. Rozema[2], Scott J. Miller[2]*, and Song Lin[1]**

[1]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY
[2]Department of Chemistry, Yale University, New Haven, CT

Catalyst-Controlled Regiodivergent Oxidation of Unsymmetrical Diols

15. ***Cory G. Walck** and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo NY

Computational Chemistry Study of Alkaline-Earth Monoborohydride Isomers

16. ***Ashlie M. Sitzer**, M. Rebecca A. Walls, Shannon E. Cooney, and Ellen M. Matson**

Department of Chemistry, University of Rochester, Rochester, NY

Synthesis, Purification, and Characterization of Tungsten-Doped Polyoxovanadate-Alkoxide Clusters

17. ***Elizabeth Holyat** and Claire Besson**

Department of Chemistry, Binghamton University, Binghamton, NY

Spectroscopic and Structural Investigations of Chromium Scorpionate Complexes

18. ***Jonas G. Simora**, Peter S. Rice, Hugh F. Foley, S. Thomas Autrey, and Bojana Ginovska*

Department of Energy Office of Science, PNNL, Richland, WA

Fine-tuning Graphene Systems for Hydrogen Storage

19. ***Matthew E. Wass*** *and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Computational Chemistry Study of Alkali Metal Monomethyls and Monoethyls

20. ***Maria G. Kim*** *and Alexey V. Ignatchenko**

Department of Chemistry, St. John Fisher College, Rochester, NY

Alkylation of 1,3,5-Tribromobenzene by Cycloheptyl Bromide via Suzuki Coupling Reaction

21. ***Nicholas J. Reilly****, Karoline E. García-Pedraza, and David F. Watson**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Ferrocene Functionalized Quantum Dot Systems as Enhanced Photocatalysts for Aqueous Hydrogen Evolution

22. ***Delila C. MacLeod, Richard J. Bouck****, Joshua Thomson, Julian Ramos, Daniel Sheibley, Sarah Glick, and Suzanne F. O'Handley**

School of Chemistry and Material Science, Rochester Institute of Technology

Diadenosine Polyphosphatases of the NUDIX Hydrolase Superfamily in *M. tuberculosis* and *M. leprae*

23. ***Evan M. Folsom*** *and Timothy M. Gregg**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Retrosynthetic Application and Analysis of Lactone-Containing Isocoumarin E

24. ***Isabella Peroni****, Catherine Larrow, and Luis Sanchez**

Department of Biochemistry, Chemistry, and Physics, Niagara University

Synthesis of Dehydroleucine Derivatives as Building Blocks for Complex Molecule Synthesis

25. ***Yaroslav Malynych*** *and Kacie R. Liwosz**

Department of Natural Science and Mathematics, D'Youville University

Manganese Dioxide Nanoparticles as Catalysts for Organic Synthesis

26. ***Robert C. Ghetiu**** *, Daniel Kamzol, and René Wilhelm*

Institut für Organische Chemie, Technische Universität Clausthal, Clausthal-Zellerfeld, NI

Camphor-derived Tetradentate Ligands: Synthesis, Iron (II) Complexation, and Catalytic Potential

27. ***Ryan Nguyen****, LeAnn Richert, and Luis Sanchez**

Department of Biochemistry, Chemistry, and Physics, Niagara University

A Bicyclic Ring Closure-Based Strategy for the Synthesis of Cage Molecule Building Blocks

28. ***Jeb Braunscheidel****, John G. Federice, and Timothy M. Gregg**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Progress Toward the Enantioselective Synthesis of Rhytismatones A and B

29. ***Sawyer A. Oppenneer****, Isabelle R. Price, Allan Jay P. Cardenas, and Thuy Thanh D. Le**

Material Science Division, Pacific Northwest National Laboratory, Richland WA

Catalytic Hydrogenation of Benzaldehyde Using Rhodium-Based Catalysts

Poster 1.

Colloidal Synthesis Dataset Development of Non-Precious Metal Oxide Electrocatalysts for Oxygen Reduction Reaction

***Olivia Wong**, Xin Wang, Rak Sreeram, Ryan Tse, and Héctor Abruña**

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY

Fuel cells and electrolyzers can provide a path for clean sustainable energy solutions to mitigate the impact of fossil fuel dependence. However, the reactions involved, particularly the oxygen reduction (ORR) and oxygen evolution (OER) reactions generally require the use of expensive precious metal catalysts such as platinum and iridium. This has prompted considerable research interest in developing alternative electrocatalysts using abundant and non-precious metals, particularly first row transition metals. Since no single non-precious metal can fully match the performance of platinum, combining multiple transition metals to exploit their synergistic interactions presents a promising strategy. A critical challenge in advancing these materials lies in generating robust synthesis datasets suitable for machine learning models, enabling predictive design and optimization of catalyst properties.

Our work addresses this gap by synthesizing and characterizing a broader set of primarily first-row transition metal oxide catalysts using colloidal synthesis methods. Applying statistical methodologies, such as Independent and Identically Distributed (IID) random variables and Design-of-Experiment (DoE) methodologies, this study systematically designs and builds a comprehensive dataset focused on the synthesis of transition metal oxide electrocatalysts. Synthesized catalysts were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy-dispersive spectroscopy (EDS), and rotating disk electrode (RDE) voltammetry experiments to provide a robust and well-defined dataset. This dataset enables rigorous machine learning analysis and predictive modeling, supporting the development of cost-effective and high-performance electrocatalysts for sustainable energy applications.

Poster 2.

Computational Chemistry Study of Alkaline-Earth Monoamide Isomers

Grace E. Baumgartner *and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Metal amides are strong bases that constitute a class of important reagents in organic synthesis. The simplest species are the metal monoamides (MNH_2) and these molecules, which are metal derivatives of ammonia, offer a way of understanding the metal-nitrogen bond at a fundamental level. Using Density Functional Theory (DFT) and several functionals with various triple and quadrupole zeta basis sets, isomers of Mg, Ca, and Sr monoamides have been investigated in their ground electronic state. Highly accurate bond lengths and angles, relative energies, dipole moments, vibrational frequencies, and other properties have been calculated for the planar MNH_2, bent HMNH, and planar NMH_2 isomers. The planar MNH_2 isomer was found to be the lowest in energy for all three metals. In addition, calculated dihedral potential energy curves reveal a relatively flat surface around the planar MNH_2 geometry and a transition state involving bridging hydrogen atoms. Calculated structural parameters for the MNH_2 species will be compared to experimental data and bonding in the various isomers will be discussed.

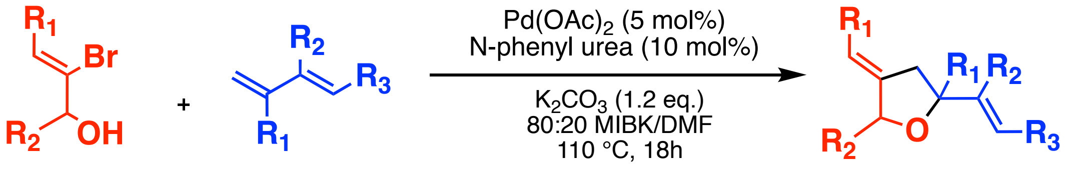
Poster 3.

Olefin Heteroannulation with Non-Aromatic Ambiphiles via Urea-Enabled Palladium Catalysis

***Brooke R. Stanley**, Shannon O'Neil, Owen E. Monteferrante, and Shauna M. Paradine**

Department of Chemistry, University of Rochester, Rochester, NY

Olefin heteroannulation, in which bifunctional (ambiphilic) and olefin reagents are coupled via palladium catalysis, enables the rapid construction of heterocyclic scaffolds. Previously, our group demonstrated that compounds derived from urea are effective ligands for palladium, promoting the heteroannulation of bromoanilines[1] and bromophenols[2] with diverse diene coupling partners. Extending this methodology to non-aromatic ambiphiles, whose reduced acidity and increased conformational flexibility can hinder the key nucleophile addition step, is not trivial and has remained a limitation of olefin heteroannulation. In this work, we show that heteroannulation by these similar conditions can be achieved with non-aromatic, acyclic ambiphiles, enabling access to sp^3-rich heterocyclic compounds. The polysubstituted THF rings that our method affords are versatile synthetic intermediates and prevalent motifs in medicinally relevant polyketide natural products[3]. This methodology is effective with a structurally and functionally diverse range of coupling partners, which make it an attractive strategy for the generation of these privileged THF compounds.



- **flexible ambiphiles that are acyclic and non-aromatic**
- **further functionalization through scaffold and substitution diversity**
- **urea ligands that create a robust and bench-stable platform**

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[1] Vaith, J.; Rodina, D.; Spaulding, G. C.; Paradine, S. M. *J. Am. Chem. Soc.* **2022**, *144*, 6667– 6673.

[2] Houghtling, K. E.; Canfield, A. M.; Paradine, S. M. *Org. Lett.* **2022**, *24* (31), 5787– 5790.

[3] R. A. Fernandes, R. S. Pathare, D. A. Gorve, *Chem. Asian J.* **2020**, *15*, 2815.

Poster 4.

Optimization of Dye-$CuAlO_2$ Films for Hydrogen Generation

***Jenna L. Davies,*[1] *Isabelle R. Prentice,*[1]** *Michael D. Clark,*[2] *Zachery A. Schmidt,*[2] *Gregory J. Lapp,*[1]
Hannah R. Dierolf,[1] *Kacie R. Liwosz*,*[1] *and David F. Watson*[2]

[1]Department of Natural Science and Mathematics, D'Youville University, Buffalo, NY
[2]Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

We prepared dye-sensitized photocathodes (DSPs) by attaching a phosphonic acid-functionalized selenorhodamine dye (3-SeP) to delafossite $CuAlO_2$ thin films. The dye 3-SeP adsorbed to $CuAlO_2$ as a mixture of monomeric and H-aggregated dyes, broadening the dye's absorption profile and enhancing the absorption of visible light. $CuAlO_2$ was synthesized by dissolving $Cu(NO_3)_2$ and $Al(NO_3)_2$ separately in distilled water, then combining together along with citric acid and ethylene glycol and then heating at various temperatures. Optimization of the synthesis of $CuAlO_2$ films was completed by varying spray coating methods followed by thermal treatment. The films were further tested through surface dye-loading experiments using diffuse reflectance spectroscopy to examine dye attachment of differing dyes and varying pH's of the electrolyte solution. Electrodes with the dye exhibited 7-to-8-fold greater reductive photocurrents than without the dye, which is evidence that hole transfer could reduce protons. In prolonged-illumination chronocoulometry experiments, our films with a supporting electrolyte reduced H^+ to H_2 with Faradaic efficiency of (43 ± 27)%. Our results highlight the potential of dye-sensitized Cu(I) delafossites as DSPs for redox photocatalysis and the production of solar fuels.

Poster 5.

Development of a Biaryl Oxidative Coupling-Based Route to the Anti-Tumor Natural Products TMC-95

***Elise Spence**, Steele Burgeson, and Luis Sanchez**

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

First isolated from the fermentation broth of *Apiospora montagnei* Sacc. TC 1093, the natural products TMC-95 A–D are of great interest because of their biological activity against the 20S proteasome. This distinctive activity makes them promising candidates as agents for the treatment of cancer. However, constructing such complex molecular structures requires many synthetic steps, which hinders their potential medical use. These active compounds feature a peptide-based structure composed of tyrosine, asparagine, a highly oxidized tryptophan, (*Z*)-1-propenylamine, and 3-methyl-2-oxopentanoic units. A particularly unusual bond is found in these natural products: a biaryl connection between the tryptophan and tyrosine residues and, as a result of this strange C–C linkage, axial chirality is observed around this bond. Our primary interest in this project is to develop chemical conditions to form this important biaryl linkage via oxidative coupling of suitable tripeptide-based building blocks. Such an oxidative coupling can make the synthetic production of TMC-95 significantly easier, by starting with the inexpensive and widely available natural amino acid units. With an easier synthetic route, TMC-95-based compounds could become viable anti-tumor drug candidates.

Poster 6.

Reduced Polytungstates in Nonpolar Environments

Aaron J. Szczepankiewicz*, *Emily R. Barry*, *and Steven H. Szczepankiewicz*

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Transition metal substituted heteropoly tungstates are well-established multi-electron reduction catalysts in polar solvents. They are also known to bind strongly with CO_2 when dissolved in nonpolar solvents. No CO_2 reduction is observed in polar solvents because the solvent molecules occupy the binding site. Similarly, direct electrochemistry in nonpolar solvents has yielded no promising results. Catalyst candidates are easily reduced in water in the presence of electrolyte. The reduced tungstates are phase-transferred intact into toluene solution with careful exclusion of oxygen. This system provides a promising means to evaluate the reactivity of the reduced tungstate with CO_2 under favorable binding conditions.

Poster 7.

Synthesis and characterization of [Fe^{II}(4-BrTp)] for use in Spin-Crossover-Based Electronic Devices

Zachary C. Ellis*, Gabrielle Shin, Alexander Ruhren, and Claire Besson**

Department of Chemistry, Binghamton University, Binghamton, NY

Spin crossover (SCO) transition metal complexes have been increasingly explored as a foundation for next-generation molecular sensors and electronic devices. Iron(II) complexes including trispyrazolylborate (Tp^-) ligands are particularly attractive candidates for these applications due to their robust magnetic properties, stability, tunability, and low cost of synthesis. In this study, we designed, optimized and refined the synthesis of a bromine-functionalized Tp^- ligand, (4-bromopyrazolyl)dipyrazolylborate (4-$BrTp^-$), and its iron(II) complex [Fe(4-BrTp)$_2$] (Figure 1, top). The structures of both ligand and complex were determined by single crystal XRD (Figure 1, bottom). The introduction of a 4-bromo substituent provides a useful synthetic handle for further modifications while still maintaining the desired SCO properties; we propose that these complexes could serve as adaptable precursors for advanced functional materials, as the bromine group allows for subsequent palladium-catalyzed cross-couplings. This strategy enables fine-tuning of electronic and steric effects through derivatization, allowing for precise control over spin-state transitions. These SCO changes can be monitored using characterization techniques including NMR and IR spectroscopy, providing insight into spin state and molecular structure through peak shifts. By using this modular approach, we aim to aid the development of next-generation switchable materials with enhanced performance and tailored functionalities, contributing broadly to the advancement of SCO materials for molecular sensing and electronic applications.

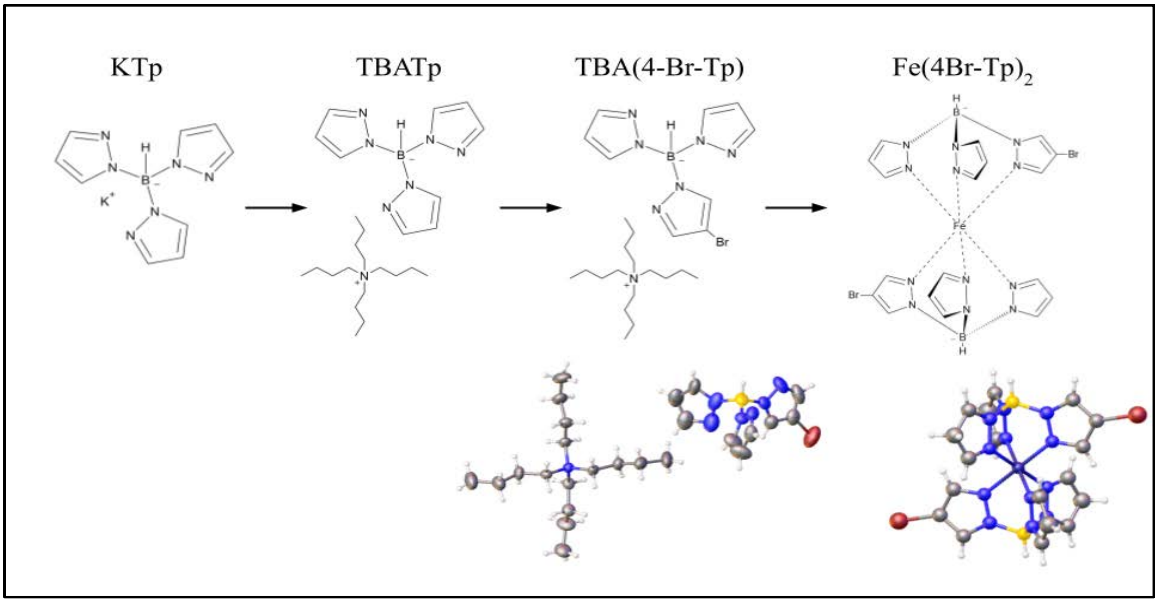


Figure 1: Synthetic route for the formation of [Fe(4Br-Tp)$_2$] (top); crystal structures of (^{n}Bu$_4$N)(4-BrTp) and [Fe(4-BrTp)$_2$] (bottom; Fe = dark blue, Br = orange, N = blue, B = yellow, C = grey, H = white).

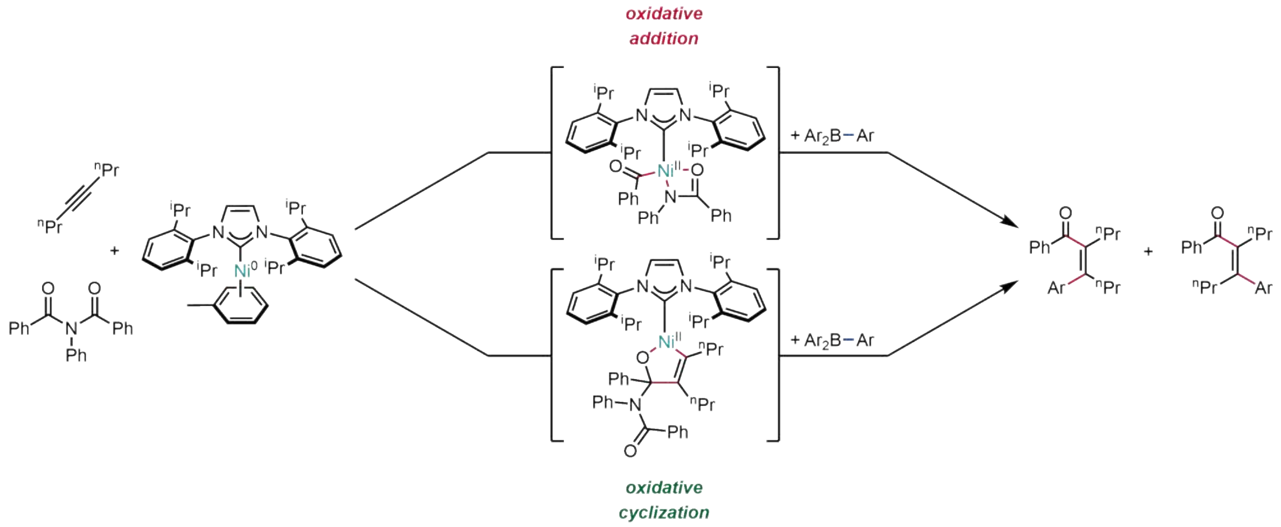
Poster 8.

Mechanistic Insight into Nickel-catalyzed Conjunctive Cross-coupling of Amides

***Matthew T. Gleason**, Kaycie Malyk, Vivek G. Pillai, and C. Rose Kennedy**

Department of Chemistry, University of Rochester, Rochester, NY

Transition metal-catalyzed conjunctive cross-coupling reactions offer a versatile way of accessing complex moieties with high atom-economic efficiency. In recent years, there has been an increased effort to develop new methodology that moves away from expensive precious metal catalysts to inexpensive, environmentally benign 3d metal catalysts, such as nickel. Nickel-catalyzed conjunctive cross-couplings have emerged over the past decade, but progress has been stymied due to the lack of mechanistic insight. This poster details the ongoing work of gaining mechanistic insight into the Ni/ N-heterocyclic carbene-catalyzed intermolecular carboacylation of amide electrophiles with alkynes. Spectroscopic observation and isolation of key catalytic intermediates serve as the basis for advancing mechanistic understanding of oxidative addition and oxidative cyclization pathways.



Poster 9.

Self-Assembled Monolayers: A Transition from Disordered to Ordered, and Their Applications in the Industrial and Biomedical Fields

Jacob P. Smeraldo *and Alexander J. Rupprecht**

Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY

Many organic molecules containing polar functional groups have the ability to bind to the passive oxide layer on a metal surface to create a one molecule thick film of organic molecules that can be referred to as a self-assembled monolayer (SAM). Most currently studied SAMs are made up of long alkyl chains containing polar functional groups and while they have been found effective at self-assembling and can be functionalized to have applications in the industrial and biomedical fields the ability of the alkyl chain to freely bend and rotate throughout space causes disorder to arise within the film which reduces the effectiveness of the SAM. As a result of these findings, our group has proposed a synthetic scheme to create a library of phenyl-based molecules which can be used as adsorbates to form SAMs and are predicted to be more ordered when deposited onto the passive oxide layer of a metal. The synthesis of the molecules will be determined using Fourier Transform IR (FT-IR) and NMR spectroscopy, the ordered nature of the SAMs after deposition will be determined using Diffuse Reflectance for Infrared Fourier Transform IR (DRIFT-IR) spectroscopy, and the effective functionalization of the SAMs after deposition will be determined using DRIFT-IR spectroscopy, electrochemical data, and biocompatibility testing.

Poster 10.

Discovering Tellurium's Reactivity: Synthetic Progress Towards a Novel Benzo-fused Telluropyrylium Chromophore

Zachary E. Holmes[1], *Matthew R. Crawley*[2], *and Lauren E. Rosch**[1,2]

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[2]Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Heavy chalcogen-containing pyrylium dyes have been studied for over 40 years for their use in biomedical imaging and photodynamic therapy. Recent reports have shined light on gaps in the understanding of the electronic and photophysical properties of this class of molecules and have begun to explore specifically tellurium reactivity. We are working to expand on these studies by exploring carbon-tellurium bonding nature through X-ray charge density measurements and other reactivity studies. Currently, our goal compound is a novel benzo-fused heavy chalcogen-containing chromophore. We report progress on a five-step synthesis from commercially available phenylacetylene. Synthetic steps include first coupling a ditelluride to an acetylenic ester, cyclization of the resulting alkene, then a subsequent methylation. The synthetic routes to the selenium analog for the goal compound and precursor molecules are reported in the literature and serve as a foundation to our synthetic pathways. Synthetic progress, structural, and photophysical characterization will be discussed.

References:
Rosch, L. E., et al. *Organometallics*, **2022**, *41* (16) 2301-2316
Kalita, N., et al. *Inorg. Chem.*, **2024**, *63* (29), 13157-13165

Poster 11.

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Haloperoxidase Biomimicry: Toward the Generation of Electrophilic Species Utilizing Xerogel-Based Transition Metal Catalysts

Alex B. Szczepankiewicz *and Corey Damon**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Vanadium haloperoxidases are naturally occurring enzymes found in species such as the fungus *Curvularia inaequalis*, a plant saprobe utilizing vanadium chloroperoxidase. In fungi and other species, the active catalyst functions to accelerate the transformation of water, hydrogen peroxide, and free halide ions into the formation of hypohalous acids. The production of hypohalous acids is of particular interest in the marine antifouling industry, as these species serve as a negative settlement cue, to discourage the settlement of fouling organisms such as algae or tubeworms. The incorporation of a catalyst into marine antifouling coatings is a promising, environmentally friendly alternative to the traditional biocides in commercial use. Silica-based xerogels present the opportunity to incorporate catalysts to produce hypohalous acids using reagents naturally present in seawater while maintaining the ability to fine–tune surface properties such as hydrophobicity. As the active site of vanadium haloperoxidases involves a highly oxidized vanadium species, the focus of this work is thus to develop a variety of xerogel-based transition-metal catalysts and measure their catalytic performance toward the generation of hypohalous acids. We have been successful in using said catalysts to oxidize both bromide and chloride under gentle, aqueous conditions using hydrogen peroxide at rates that have exceeded traditional organochalcogen catalysts. To date, the most promising candidates have arisen from titanium, tungsten, vanadium, or molybdenum integrated in a silica framework. Current work includes focusing on fine-tuning the xerogel matrix to ensure incorporated metals remain sequestered and developing more monoliths with varying promising candidates.

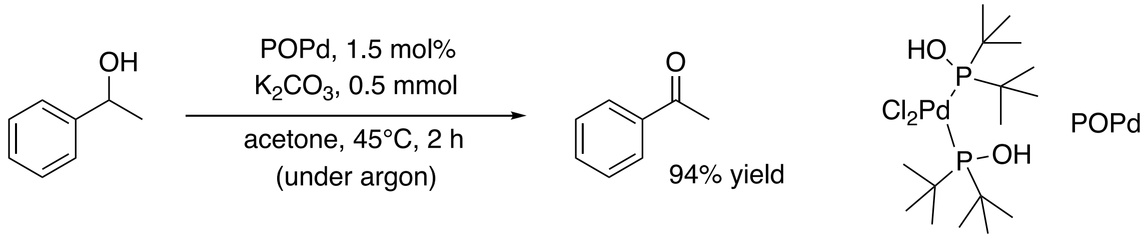
Poster 12.

Green Anaerobic Oxidation of Alcohols

***Dhani V. Slaughter**, Noelle M. Linenfelser, and Karen E. Torraca**

Chemistry Department, Houghton University, Houghton, NY

The development of a greener process has been investigated for palladium catalyzed anaerobic oxidation reactions. The initial reaction conditions for this research were determined by previous research students using 1 mmol of 1-phenylethanol as the model compound: 2.5 mol% $Pd(OAc)_2$, 2 mmol sodium percarbonate, and 2 mL anhydrous propylene carbonate at 80°C for 20 h. Although this reaction averaged 89.6% yield of the product based on an internal standard, propylene carbonate proved to be difficult to separate from the product. A multitude of catalysts, bases, additives, emulsifiers, solvents and reaction conditions were explored to optimize the reaction conditions. Initial reactions focused on the use of water as a solvent. Water resulted in loss of the starting alcohol with poor yield of the expected product. Methanol as a solvent resulted in moderate yields. Acetone produced the most consistent and highest yields, but only when using POPd as the catalyst. Potassium carbonate as the base allowed for the quickest reaction time. Final new optimized conditions for 1 mmol of 1-phenylethanol include 1.5 mol% POPd, 0.5 mmol potassium carbonate, and 2 mL anhydrous acetone at 45°C for 2 hours.



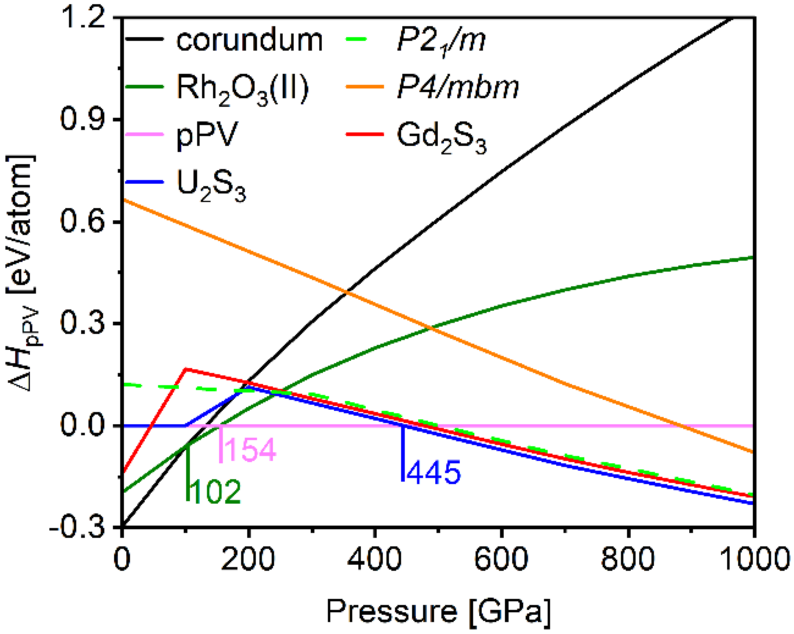
Poster 13.

Computational Investigation into Aluminum Oxide (Al_2O_3) at Planetary Conditions

***Amelia Kelly**, Stefano Racioppi, and Eva Zurek**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Aluminum Oxide (Al_2O_3), also known as alumina, is an abundant component in the interior of rocky planets. It plays an important role in the geochemistry and geodynamics of planetary bodies, such as Earth, Mars, and similar exoplanets. However, few theoretical and experimental studies have investigated the physical-chemical behavior of this compound above 500 GPa, and none have examined the effect of aluminum's core electrons on the stability and properties of its compounds. This computational study investigates aluminum oxide from 0 to 1 TPa, assessing the role of aluminum's core electrons on the stability of high-pressure Al_2O_3 crystalline phases. Ab initio Density Functional Theory (DFT) calculations were performed with the Vienna Ab initio Simulation Package (VASP) and meta-generalized gradient approximations (meta-GGAs). Structural optimizations were conducted to determine 0 K phase diagram of Al_2O_3 up to 1 TPa. Additionally, crystal structure searches at 500 GPa and 1 TPa, using the XtalOpt evolutionary algorithm-based code, identified a previously unreported stable monoclinic phase ($P2_1/m$) with a formula unit of 6, which may have been overlooked in prior studies due to methodological limitations. These findings offer initial insights into how aluminum's outer core electrons influence Al_2O_3 stability at high pressures. Further phonon calculations are on the way to determine and refine the *P*-*T* phase diagram of this important planetary compound.



Poster 14.

Catalyst-Controlled Regiodivergent Oxidation of Unsymmetrical Diols

Reginald A. Annor[1]*, Samson B. Zacate*[1]*, Jonas Rein*[1]*, Soren D. Rozema*[2]*, Scott J. Miller*[2]**, and Song Lin*[1]***

[1]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY
[2]Department of Chemistry, Yale University, New Haven, CT

In this work, we use aminoxyl-peptide conjugates to catalyze the regiodivergent oxidation of unsymmetrical diols. Our group recently developed modular aminoxyl-peptide conjugates as catalysts for the oxidative desymmetrization of meso-diols to form chiral lactones. In this system, an achiral aminoxyl radical core was coupled with a small chiral peptide. To account for the notable enantioselectivity observed across a broad range of meso-diol substrates, we proposed a stereochemical model featuring a strong two-point binding of the diol to the catalyst. While one alcohol reacts with the active oxoammonium catalytic unit, the other engages in hydrogen bonding with the peptide backbone. To apply the framework to the selective oxidation of unsymmetrical diols, we sought to modify the aminoxyl-peptide catalysts via two distinct avenues. Given that the steric and electronic properties of aminoxyl radicals have a profound influence on their reactivity, we aimed to modify the catalyst core to modulate substrate-controlled selectivity bias. We envisioned that a sterically congested core would favor the oxidation of the more accessible site, whereas a less hindered core would result in unbiased oxidation of both alcohols. Thus, by further tuning the structure of the peptide backbone to implement noncovalent substrate binding, we achieved catalyst control that either reinforces or overrides the intrinsic steric bias, leading to oxidation of either the less hindered or the more hindered alcohol in high selectivity.

Poster 15.

Computational Chemistry Study of Alkaline-Earth Monoborohydride Isomers

Cory G. Walck *and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo NY

Metal borohydrides are a class of compounds with high hydrogen densities that are currently being investigated for their hydrogen fuel storage capabilities. The simplest molecules are the metal monoborohydrides (MBH_4) and these species offer a way of understanding the metal-borohydride bond at a fundamental level. Several isomers are possible, including those with varying numbers of hydrogen atoms acting as a bridge between the boron and metal atoms. Density Functional Theory (DFT), including several functionals and basis sets, was used to calculate the energies, geometric properties, vibrational frequencies, dissociation energies, rotational constants, and ionic character for several isomers of alkaline-earth metals monoborohydrides. For magnesium, calcium, and strontium, the tridentate isomer was found to be the lowest in energy by all calculation methods. The bidentate and monodentate isomers were found to be transition states and a stable hydrido-borane isomer was also discovered for each of these metals. Calculated molecular properties will be compared between isomers of a particular metal, as well as between metals for a particular isomer.

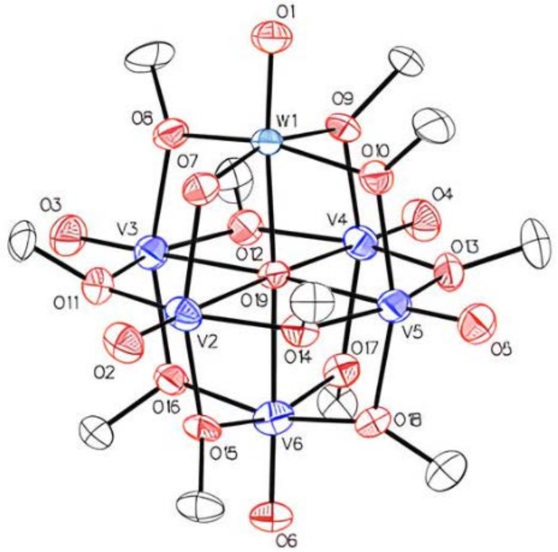
Poster 16.

Synthesis, Purification, and Characterization of Tungsten-Doped Polyoxovanadate-Alkoxide Clusters

Ashlie M. Sitzer, *M. Rebecca A. Walls, Shannon E. Cooney, and Ellen M. Matson**

Department of Chemistry, University of Rochester, Rochester, NY

Understanding and controlling the structure of heterometal-substituted polyoxovanadate (POV)-alkoxide clusters is crucial for advancing their applications in redox-active chemistry, catalysis, and energy storage. However, previous efforts to isolate and characterize tungsten-doped POV-alkoxide clusters have proved challenging as they are formed in mixtures. This has limited the ability to study their intrinsic properties and potential reactivity, creating a gap in the general studies of these heterometal-substituted POV-alkoxide clusters. To address this challenge, we aim to refine the synthesis and purification of tungsten-doped POV-alkoxide clusters to obtain well-defined, pure compounds. We employ simplified starting materials and various reductants to control cluster formation, alongside optimized purification techniques such as column chromatography, Soxhlet extraction, and controlled crystallization. Our findings show that these modifications reduce cluster distribution, enhancing selectivity. Notably, we have successfully isolated and characterized a mono-tungsten-doped cluster, $WV_5O_8(OCH_3)_{11}$, using X-ray crystallography. This begins to provide insight into structure-property relationships within these systems. By expanding this library of well-defined tungsten-doped clusters, this work contributes to the broader understanding of redox-active materials. These clusters will be used to explore proton-coupled electron transfer as well as oxygen atom transfer, informing future applications in catalysis and energy storage.



Poster 17.

Spectroscopic and Structural Investigations of Chromium Scorpionate Complexes

Elizabeth Holyat *and Claire Besson**

Department of Chemistry, Binghamton University, Binghamton, NY

Scorpionate ligands, known for their strong yet flexible coordination to metal centers, play a crucial role in tuning electronic and magnetic properties in transition metal complexes. Tris(pyrazolyl)borate (Tp^-) ligands, a well-studied class of scorpionates, provide a stabilizing environment that can support a range of oxidation and spin states. This research focuses on the synthesis and characterization of chromium scorpionate complexes, particularly chromium with two tris(pyrazolyl)borate ligands. A $[Cr^{III}Tp_2]^+$ complex with $[Cr^{III}TpCl_3]^-$ as the counterion (Figure 1) has been synthesized and characterized using X-ray crystallography as well as infrared, UV-Vis, and fluorescence spectroscopies to investigate its structural and electronic properties. Ongoing efforts are focused on synthesizing $[Cr^{III}Tp_2]^+$ complexes with different counterions, such as chloride and nitrate, to explore how counterion identity influences electronic structure and emission behavior. A recent study on Cr^{II} complexes in trigonal antiprismatic environments, featuring ligands structurally similar to Tp^-, have shown spin-crossover properties and unexpected air stability, despite requiring inert-atmosphere synthesis.[1] These findings suggest that $Cr^{II}Tp_2$ may also exhibit spin-crossover behavior. Furthermore, incorporating electron-withdrawing nitro groups in a complex like $Cr^{II}(3\text{-}NO_2Tp)_2$ may stabilize the Cr^{II} oxidation state, reducing its tendency to oxidize to Cr^{III} while maintaining the potential for spin-crossover. Exploring how oxidation state, counterion identity, and ligand modifications affect electronic structure will offer broader insights into chromium scorpionate chemistry and its applications in catalysis, photochemistry, and molecular magnetism.

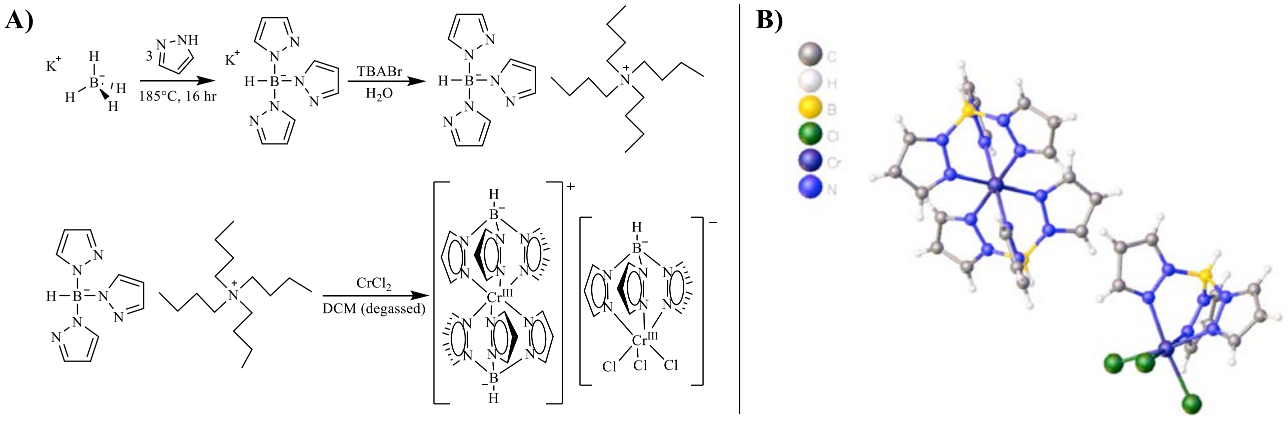


Figure 1. **A)** Synthesis of $[Cr^{III}Tp_2]^+[Cr^{III}TpCl_3]^-$ **B)** Crystal structure of $[Cr^{III}Tp_2]^+[Cr^{III}TpCl_3]^-$

[1] Liu et al. Trigonal Antiprismatic Mononuclear Cr(II) Spin-Crossover Complexes. *Inorganic Chemistry Frontiers,* **2025**, *12* (6), 2236-2244. DOI:10.1039/d4qi02973a.

Poster 18.

Fine-tuning Graphene Systems for Hydrogen Storage

Jonas G. Simora*, *Peter S. Rice, Hugh F. Foley, S. Thomas Autrey, and Bojana Ginovska*

Department of Energy Office of Science, PNNL, Richland, WA

Interest surrounding carbon sorbent materials, such as graphene, as a medium for solid-state hydrogen (H_2) storage has grown in recent years as the United States look to transition toward green energy. One of the methods, which would allow for stable H_2 storage at ambient temperatures involves doping of these materials with nitrogen. The project aims to fine tune the electronic properties of graphene systems through doping with nitrogen (N) atoms for the purposes of increasing the efficiency of hydrogen storage. This fine tuning involves the simulation of graphitic and pyridinic N defects on both planar and rippled graphene systems. We were able to determine the relative stability of these defects by calculating the formation energy of each defect being modeled. From these calculations, we were able to determine that the rippled nature of graphene has a significant impact on the doping stability of the system. Increasing stability of these (N) doped graphene systems, even with defects, would enable increased hydrogen storage efficiency; helping to solve this problem associated with using hydrogen as a source of energy.

Poster 19.

Computational Chemistry Study of Alkali Metal Monomethyls and Monoethyls

Matthew E. Wass *and Phillip M. Sheridan**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

Organometallic compounds are molecules that contain a metal-carbon bond. These species are important in organic synthesis as they can be used for addition and substitution reactions, be used in the preparation of strong bases, and be used as catalysts. Simple organometallics, such as metal monomethyls and monoethyls can serve as model compounds to better understand the metal-carbon bond. This research focused on alkali metal monomethyls and monoethyls through computational analysis with the Gaussian 16 computational software package. Computational analyses were conducted for lithium, sodium, potassium monomethyl and monoethyl compounds. Electron correlation methods such as Density Functional Theory, Møller–Plesset Perturbation Theory, and Coupled-Cluster with Single, Double, and Perturbative Triple Excitations Theory were conducted for their respective sophistication, and the 6-311G++ (3df, 2pd) and aug-cc-pVTZ basis sets were applied to the mentioned methods for comparison of computational results. Molecular properties, such as bond lengths and angles, relative energies, dipole moments, vibrational frequencies, hyperfine parameters, and bond orbital overlap were calculated. These molecular properties were compared by computational methods and by molecules to gain insight into the chemical stability and bonding character of these prototypical organometallic molecules. From these comparisons it was determined that the metal-carbon bond is largely ionic, more so for monomethyls than monoethyls, the carbon bonded to the metal is approximately sp^3 hybridized, and there is no significant difference for the bond rotational barrier between carbons for ethane and alkali monoethyl molecules.

Poster 20.

Alkylation of 1,3,5-Tribromobenzene by Cycloheptyl Bromide via Suzuki Coupling Reaction

Maria G. Kim *and Alexey V. Ignatchenko**

Department of Chemistry, St. John Fisher College, Rochester, NY

Carbon has several known allotropes, graphite, diamond, amorphous; there are also cylindrical nanotubes and spherical fullerenes. Scientists are trying to make another hypothetical allotrope that is called schwarzite, a 3d porous material made out of carbon heptagons, which does not exist in nature. Scientists failed to make it similar to the preparation of nanotubes, fullerene, but there is hope to make Schwarzites through bottom up synthesis. When graphene planes are attached to each other they form graphene. When seven membered rings are incorporated in graphene structure, it starts curving and may form a 3d structure. Thus, it will require some hexagons in the graphene to be replaced with heptagons. For that reason, cycloheptane needs to be combined in trimers; one of the molecules is 1,3,5-tricycloheptyl benzene.

This molecule was prepared by Suzuki coupling reaction between 1,3,5-tribromobenzene and cycloheptane-boronic acid. Commercially available bromocycloheptane was converted into boronic acid via a Grignard reaction synthesis. For the Suzuki coupling reaction catalyzed by palladium, the following were tried: two different palladium catalysts, $Pd(PPh_3)_3$ and $Pd(dppf)Cl_2$; two different solvents, THF and DMFA; and three different bases, triethylamine, potassium carbonate, and dimethylformamide. After many trials it was found that potassium ethoxide and solvent THF works best. The product was purified and isolated by column chromatography and characterized by ^{1}H and ^{13}C NMR. This compound will be used as the precursor for making the building blocks for the construction of schwarzites.

Poster 21.

Ferrocene Functionalized Quantum Dot Systems as Enhanced Photocatalysts for Aqueous Hydrogen Evolution

Nicholas J. Reilly, *Karoline E. García-Pedraza, and David F. Watson**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

CdSe quantum dots (QDs) are well documented, capable photocatalysts for green energy-forward reactions. Unfortunately, upon absorbing light, these materials suffer photodeterioration and inefficient radiative recombination because of hole accumulation and undesirable electron-hole dynamics. 6-(ferrocenyl)hexanethiol (FcC_6SH) ligands attached to the quantum dot surface are known to induce the rapid separation of electron holes to their oxidizable Fe (II) cores, hypothetically minimizing these issues. In this study, the effect these ligands have on the quantum dot system's photostability and hydrogen gas evolution rates in acidic aqueous solutions was investigated. Oleic-acid CdSe QDs are synthesized by hot injection and functionalized with FcC_6SH ligands in organic solutions. The attachment of hole-removing ligands is followed by intense photoemissive quenching, characterized by emission drops in bulk and time-correlated fluorimetry, often with total quenching >90%. QD samples are interfaced with an acidic aqueous electrolyte to facilitate the photoelectrochemical reduction of protons to hydrogen gas as a green fuel alternative. These systems are constructed using a 3-electrode setup, with a potential applied across the QD working and platinum counter electrodes. Compared to control oleic-acid QD samples, this system has been shown to enhance hydrogen gas production over a prolonged illumination by upwards of 300% in some trials.

Poster 22.

Diadenosine Polyphosphatases of the NUDIX Hydrolase Superfamily in *M. tuberculosis* and *M. leprae*

Delila C. MacLeod, Richard J. Bouck*, Joshua Thomson, Julian Ramos, Daniel Sheibley, Sarah Glick, and Suzanne F. O'Handley**

School of Chemistry and Material Science, Rochester Institute of Technology, Rochester, NY

M. tuberculosis contains 11 potential Nudix hydrolases, and we are characterizing these enzymes as potential novel antibiotic targets. The diadenosine polyphosphatases ($\mathrm{Ap_nAase}$) are a family of enzymes within the Nudix hydrolase superfamily. In *M. tuberculosis* there is the primary (more active) Nudix $\mathrm{Ap_nAase}$ and the secondary Nudix $\mathrm{Ap_nAase}$. There are also orthologs of these two $\mathrm{Ap_nAase}$ in *M. leprae*. The diadenosine polyphosphatases from *Legionella pneumophilia* and *Bartonella bacilliformis* have been found to be important in each pathogen's ability to invade its host cells. It is of interest to know whether these enzymes act in the same way in *M. tuberculosis* and *M. leprae*. If they are all found to be involved in invasiveness and thus in virulence, then these enzymes could be novel antibiotic targets. We have cloned and overexpressed each protein and have subcloned each into a HisTag vector to optimize purification. The *M. tuberculosis* enzymes have been purified and their $\mathrm{Ap_nAase}$ activity has been characterized. The primary $\mathrm{Ap_nAase}$ has a second domain, and thus to finish the characterization of this enzyme, we are analyzing this second domain for activity. The *M. leprae* enzymes express too insolubly to purify and characterize, and thus we are working on increasing the expression of soluble protein so that we can study these enzymes as well; currently, we know that they each have $\mathrm{Ap_nAase}$ activity (in the crude extract) above that of *E. coli* enzymes alone. Supported by an NIH AREA grant, a CUR-Goldwater Mentor Award, and a Rochester Academy of Science grant.

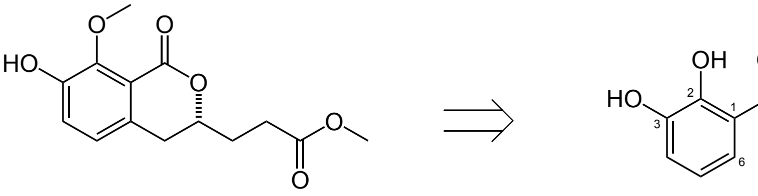
Poster 23.

Retrosynthetic Application and Analysis of Lactone-Containing Isocoumarin E

Evan M. Folsom *and Timothy M. Gregg**

Department of Chemistry and Biochemistry, Canisius University, Buffalo, NY

A novel metabolite, Isocoumarin E, isolated from a *Penicillium* fungus, was reported in 2019. This chiral molecule was reported to have insecticidal activity against cotton bollworm larvae. The absolute configuration of the natural product was assigned by correlation of CD data with calculation, so enantioselective total synthesis has the potential to confirm the stereochemistry. Our synthesis strategy focuses on elaborating an aromatic ring with 4 substituents--2 with oxygens and 2 with carbon groups. The approach we are investigating is selective bromination of a suitable 2,3-dihydroxybenzaldehyde derivative, which could then be elaborated with the needed 4th carbon chain through metalation and alkylation. The chirality could be introduced at a late stage by stereoselective ketone reduction, so our initial aim is a racemic synthesis. We describe protection and bromination reactions aimed at carbon-6 of this benzaldehyde, with varying results. These studies have led to a broader investigation of aromatic ring functionalization in pursuit of site selectivity.



Isocoumarin E

Poster 24.

Synthesis of Dehydroleucine Derivatives as Building Blocks for Complex Molecule Synthesis

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This project aims at optimizing the preparation of dehydroleucine-based compounds and using them to explore various subsequent chemical transformations. These building blocks could prove useful in the synthesis of natural products, such as the members of the celogentin family. Additionally, they could serve as stable precursors for vinylglycine derivatives. The unusual amino acid vinylglycine and a number of related compounds have been studied throughout the years for their special reactivity and involvement in certain biological processes. Given the presence of an alkene moiety, the structures can be manipulated through a variety of chemical reactions. While the preparation of vinylglycine itself has been extensively investigated in the past, its production is still problematic due to its sensitivity to racemization and isomerization, which renders key steps irreproducible during its synthesis and the preparation of derivatives. We propose that appropriately substituted dehydroleucine-based building blocks may be safe from decomposition and could serve as shelf-stable precursors to valuable materials. Our progress in these endeavors will be presented.

Poster 25.

Manganese Dioxide Nanoparticles as Catalysts for Organic Synthesis

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Manganese dioxide (MnO_2) nanoparticles have emerged as promising catalysts for organic synthesis due to their high surface area, tunable oxidation states, and environmentally friendly characteristics. In this study, we investigate the synthesis and catalytic applications of MnO_2 nanoparticles, employing both room-temperature and high-temperature methods. Preliminary investigations into the catalytic activity of MnO_2 nanoparticles in the organic transformations of styrene and acetylacetone have shown encouraging results. Thin-layer chromatography (TLC) and UV-Vis analysis indicate that MnO_2 nanoparticles effectively mediate key reaction steps. Future work will concentrate on refining the synthesis of MnO_2 nanoparticles to tailor their catalytic properties, utilizing advanced characterization techniques such as nuclear magnetic resonance (NMR), X-ray Absorption Near Edge Structure (XANES), while additional kinetic studies will be employed to further elucidate their mechanistic role in catalysis. The development of sustainable and efficient MnO_2-based catalytic systems holds significant potential for green chemistry applications.

Poster 26.

Camphor-derived Tetradentate Ligands: Synthesis, Iron (II) Complexation, and Catalytic Potential

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We present the synthesis of camphor-based amine ligands, and their Iron (II) triflate complexes, along with an analysis of their catalytic activity. Starting from camphoric acid, we synthesized a series of seven tetradentate amine ligands. Their Iron (II) complexes, pre-isolated or prepared in situ, showed catalytic activity towards the enantioselective addition of 1-methylindole to an α,β-unsaturated ketone. With our optimized conditions, we were able to achieve up to 30% enantiomeric excess. We found that lower temperatures promote higher enantiomeric excess, and that secondary and tertiary amine complexes exhibit comparable catalytic activities. We used Nuclear Magnetic Resonance Spectroscopy and Gas Chromatography/Mass Spectrometry to characterize the compounds, and chiral High-Performance Liquid Chromatography to determine enantiomeric excess. This strategy leverages the natural abundance of camphor as an abundant and cost-effective precursor for chiral ligand design.

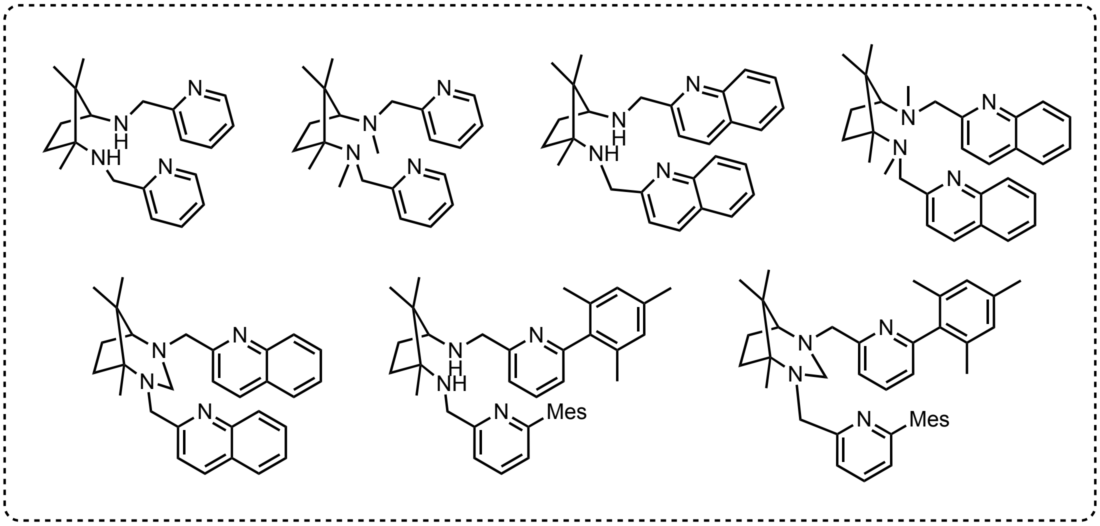

Figure 2. The 7 camphor-based ligands synthesized.

Poster 27.

A Bicyclic Ring Closure-Based Strategy for the Synthesis of Cage Molecule Building Blocks

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Platonic hydrocarbons and highly symmetric cage molecules have attracted the attention of chemists for decades. The first total synthesis of dodecahedrane, the simplest hydrocarbon with full icosahedral symmetry, more than thirty years ago was a remarkable and notorious achievement in organic chemistry. Still to date, however, the preparation of such compounds involves lengthy processes. Exploiting the elements of symmetry of the target cage molecules, as a tactic to minimize the necessary synthetic steps, is especially desirable. We noticed that building blocks containing fused five-membered rings have been the central theme of a number of studies related to cage molecules. The idea of synthesizing symmetric compounds using polycyclizations, cycloadditions, and domino reactions continues to appear, even in very recent reports, but the preparation of the required substrates for such transformations has been generally unsuccessful. The present project offers an alternative strategy for the synthesis of C_2-symmetric cage molecule building blocks, which is based on a bicyclic ring closure. Our approach and progress will be presented.

Poster 28.

Progress Toward the Enantioselective Synthesis of Rhytismatones A and B

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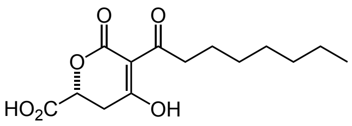
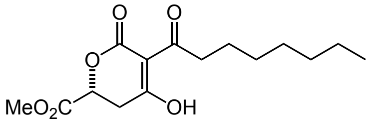
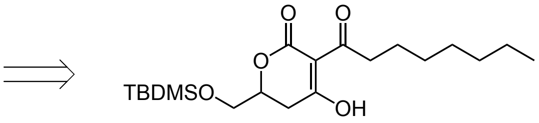
Rhytismatones A and B are produced by an unknown fungus of the Rhytismataceae family. The organism was found as an endophyte in healthy needles of *P. mariana* (black spruce). Rhytismatone B exhibited moderate antifungal activity. Neither compound has been the target of laboratory synthesis, despite the potential this would have to confirm the absolute configuration of these chiral metabolites. Our previous work on a racemic synthesis of these compounds has identified a β-elimination decomposition pathway at the chiral lactone carbon. Our current efforts focus on avoiding this presumably E1cb decomposition by approaching the final structure with a protected primary alcohol.



Rhytismatone A



Rhytismatone B



Poster 29.

Catalytic Hydrogenation of Benzaldehyde Using Rhodium-Based Catalysts

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Improving our ability to recycle biomass and waste products has become an integral focus in research due to the global energy crisis. Catalysis is a leading field in harnessing the potential energy in biomass and waste products. Hydrogenation reactions are one such avenue which can be scaled up to industry level. These catalytic reactions call for a cheap, recoverable, and efficient catalyst. Rhodium catalysts, while expensive, show great promise. To get around the price, nanometer-sized heterogeneous rhodium catalyst loaded on a titania solid support was studied in the efficiency of benzaldehyde hydrogenation as a model substrate. The reaction pathway was proposed for the rhodium nanoclusters on titania from computations and isotope labelling experiments. The pathway showed the need for multiple coordination sites for the catalyst, which led to research into the optimal number of rhodium binding sites on a molecular catalyst. Three complexes, from one to three rhodium sites, were loaded onto titania support and studied to increase efficiency and overall conversion of benzaldehyde.

NOTES: