The 1st Global Inorganic Discussion Weekday Virtual Poster Competition

#gidw2020

On Twitter, July 9th and 10th, 2020

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A note from the organizers…

We welcome you to the inaugural #gidw2020 virtual poster event – a 48 h online symposium hosted on Twitter. This poster event was spurred on by the success of our virtual lecture series (Global Inorganic Discussion Weekdays or GIDW, for short), which brings the inorganic (organometallic, main-group, materials, etc.) community together online! The name, GIDW is an homage to the popular regional conferences known as Inorganic Discussion Weekends that occur routinely in the US and Canada (and around the world with other names).

Given the current social distancing policies and travel restrictions, many of our community's standard conferences have been cancelled, preventing us from sharing our progress in science. To overcome scientific isolation and to continue celebrating our advances in inorganic chemistry, we have now organized 15 weeks of online seminars, comprising 56 speakers from Canada, USA, UK, Taiwan, Germany, France, Belgium, Germany, Israel, to name a few.

For this poster event, we would like to thank our sponsors: CIC, CSC-ID, The Wilkinson Charitable Trust, Dalton Transactions and deGruyter publishing for prizes as well as our panel of judges who will be engaging with our presenters over the next 48 h. We also thank all of our participants for submitting an abstract and the inorganic community for their continued support.

Best wishes,

Marcus W. Drover
Assistant Professor
University of Windsor
www.marcuswdrover.weebly.com
marcus.drover@uwindsor.ca
Twitter: @marcuswdrover

Saurabh Chitnis
Assistant Professor
Dalhousie University
www.chitnislab.ca
Saurabh.chitnis@dal.ca
Twitter: @chitnislab

Poster List

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***** For ease in creation of this booklet, co-authors have been omitted from abstracts.***

P1. New self-assembled hetero-metallomacrocycles as biomolecular probes and therapeutics

Stephen Aderinto
University of Sheffield, Sheffield, United Kingdom
Graduate Student
Advisor(s): Prof. Jim A Thomas

https://twitter.com/AderintoStephen
@AderintoStephen

The ability of self-assembled, kinetically-inert, water-soluble homo- and hetero-metallomacrocycles constructed from kinetically-inert d^6-cations and possessing highly-structured binding pockets made up of hydrophobic aromatic residues to bind DNA in biologically-relevant conditions has been explored, leading to the synthesis of Complex 1, the first-ever reported tetranuclear $Ru(II)_2Re(I)_2$, heteroleptic polypyridyl complex, which functions as a DNA-targeting sensitizer for PDT.

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P2. Exploring New Reaction Partners Towards the Activation Phosphine Gas (PH_3 (g))

Jeanette Adjei
Western University, London, Canada
Graduate Student
Advisor(s): Paul J. Ragogna & Michael A. Kerr

https://twitter.com/jeanette_adjei
@jeanette_adjei

This project aims to expand the scope of PH_3 chemistry towards the synthesis of new and valuable organophosphorus compounds for use in catalysis and metal coordination. Hydrophosphination reactions were used to explore the ringing opening of vinylcycloprapane and the P-H bond addition of commercially available natural products. Primary and secondary phosphines were initially used to develop the methodology of these reactions before exploring the activation of PH_3.

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P3. Synthesis, characterisation and properties of tris(3,5-difluorophenyl)borane

Mashael Alharbi
Cardiff University, Cardiff, United Kingdom
Graduate Student
Advisor(s): Dr. Rebecca Melen

https://twitter.com/Mashaelmusaad
@Mashaelmusaad

Due to extensive applications of Lewis acid boranes such as $B(C_6F_5)_3$, this work intends to synthesize novel Lewis acidic compounds.[1] These will be explored in a wide range of reactions, including small molecule activation and frustrated Lewis pair catalysis. Tris(3,5-difluorophenyl)borane has been synthesized and characterized by multinuclear NMR, mass spectroscopy, and XRD. The Lewis acidity has been determined using both the Gutmann Beckett method and the Childs' method.

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4- Ménard, G.; Stephan, D. W. *J. Am. Chem. Soc.* **2010**, 132, 1796-1797.

P4. The role of porphyrin peripheral substituents in determining the reactivities of ferrous nitrosyl species

Sk Amanullah
Indian Association for the Cultivation of Science, Kolkata, India
Graduate Student
Advisor(s): Prof. Abhishek Dey

https://twitter.com/SkAmanullah
@SkAmanullah

$\{FeNO\}_7$ is an intermediate common to the catalytic cycles of Cd1NiR (nitrite to NO) and CcNiR (nitrite to NH_4^+), heme-based NiRs, and its reactivity varies dramatically in these enzymes.[1,2] A series of iron porphyrinoids, designed to model the electron-withdrawing peripheral substitution as well as the saturation present in heme d^1 in Cd1NiR, and their NO adducts were synthesized and their properties were investigated. The detailed analysis explains the difference between PCET vs NO release.[3]

1. Averill, B. A. *Chem. Rev.* **1996**, 96 (7), 2951-2964
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P5. Iron Amino-phenolate Complexes for CO_2 Activation: Selectivity Control in Ligand Design

Kori Andrea
Memorial University, St John's, Canada
Graduate Student
Advisor(s): Dr Francesca Kerton

http://twitter.com/koriandrea
@koriandrea

We have recently reported a collection of iron (III) amino-phenolate complexes active towards the selective production of either cyclic or polycarbonates from epoxides and CO_2. Selectivity towards either product was found to be dependent both the nature of the phenolate donor, electronics and coordination geometries. During coupling reactions, those complexes in a square pyramidal geometry undergo an epoxide deoxygenation step leading to the corresponding bridged-oxo species.

1. Andrea, K. A.; Brown, T. R.; Murphy, J. N.; Jagota, D.; McKearney, D.; Kozak, C. M.; Kerton, F. M. *Inorg. Chem.*, **2018**, 57, 13494-13504.
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P6. Unexpected Reactivity of Structurally Diverse, Neutral, Hypervalent P Compounds

Nayanthara Asok
York University, Toronto, Canada
Graduate Student
Advisor(s): Dr. Thomas Baumgartner

https://twitter.com/NayantharaAsok
@NayantharaAsok

Dithienophospholes provide an interesting conjugated framework towards the synthesis of neutral pentavalent phosphorus compounds with FLP characteristics. These hypervalent compounds acquire a square pyramidal structure that is highly unusual for pentavalent phosphorus species. This peculiar geometry imparts interesting chemical properties that will be highlighted in this contribution.

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3. Osman, F.H.; El-Samahy, F. A. Reactions of α-Diketones and o-Quinones with Phosphorus Compounds. *Chem. Rev.* **2002**, 102, 629.
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7. Maskey, R.; Schädler, M.; Legler, C.; Greb, L. Bis(perchlorocatecholato)silane - A Neutral Silicon Lewis Super Acid. Angew .Chem. Int. Ed. **2018**, 57, 1717.
8. Greb. L. Lewis Superacids: Classifications, Candidates, and Applications. *Chem. Eur. J.* **2018**, 24, 17881.

P7. Photocatalytic degradation of 2,4 Dichlorophenol by the Nickel Zinc ferrite graphene oxide nanocomposite

Collen Bapiro
Midlands State University, Harare, Zimbabwe
Undergraduate Student
Advisor(s):

https://twitter.com/firebapiro
@firebapiro

The widespread use of chemicals in manufacturing industries and their frequent release into the environment is the major cause of pollution, worldwide. Inorganic chemistry can be used to synthesize compounds that degrade water pollutants.

P8. Electrochemistry and NMR Experiments of Reactions Containing Nickel(II) Complexes and CO_2 in Methanol

Zaira Barrera
University of California, Irvine, Irvine, USA
Undergraduate Student
Advisor(s): Jenny Y. Yang

https://twitter.com/zjbarrera
@zjbarrera

Reducing CO_2 to formate is a way to recycle it into a sustainable fuel. NMR and CV experiments were conducted to observe the reactivity of [Ni(dmpe)2][PF6]$_2$ & to see if [HNi(dmpe)$_2$][PF$_6$] reacts with CO_2 to produce formate in MeOH. Formate was seen at 8.5 ppm after adding CO_2 to the Ni hydride. Moreover, CV experiments with [Ni(dmpe)$_2$][PF$_6$]$_2$ under N_2 revealed that at low scan rates, irreversible formation of the Ni hydride occurred. At high scan rates, a return of the Ni(II/0) peak was observed.

1) Miedaner, A.; DuBois, D. L.; Curtis, C. J.; Haltiwanger, R. C. *Organometallics* **1993**, 12 (2), 299-303.
2) Tsay, C.; Livesay, B. N.; Ruelas, S.; Yang, J. Y. *J. Am. Chem. Soc.* **2015**, 137, 44, 14114-14121.

P9. Polynuclear Lanthanide-Diketonato Clusters: Catalytic Hydroboration of Carboxamides and Esters

Deepika Bedi
Texas Tech University, Lubbock, USA
Graduate Student
Advisor(s): Prof. Michael Findlater

https://twitter.com/deepika2705
@deepika2705

Catalytic reduction of carboxamides into their corresponding amines is an attractive but extremely challenging transformation. We have shown the direct deoxygenation of carboxamides using earth-abundant lanthanum catalysts in the presence of HBPin, delivers good to excellent yields of amines. The reaction was screened for a myriad of substrates and shows excellent functional group tolerance. Furthermore, this strategy was successfully employed to a broad range of esters.

P10. Umpolung of P-H Bond Activation for Hydrophosphination

Roman Belli
University of Minnesota, USA
Post-doctoral Fellow
Advisor(s): Lisa Rosenberg

https://twitter.com/belli_roman
@belli_roman

Efforts to develop a hydrophosphination catalyst system based on complexes that contain phosphenium ligands is described. A key step in this proposed novel catalysis is activation of a P-H bond via hydride abstraction, which we utilized to prepare phosphenium complexes from their respective secondary phosphine precursors. The viability of the additional steps for this proposed catalysis, electrophilic P-C bond formation and hydride transfer, are demonstrated even for substrates such as ethylene.

P11. Pushing the Lewis Acidity Boundaries of Boron Compounds with Non-Planar Triarylboranes Derived from Triptycenes

Ali Ben Saida
University of Namur, Namur, Belgium
Graduate Student
Advisor(s): Berionni Guillaume

https://twitter.com/ali_bensaida
@ali_bensaida

Bending the archetypal planar trigonal boron atom environment of triarylboranes results in exceptional enhancement of the boron Lewis acidity without requiring electron-withdrawing groups. The bora-phosphatriptycene, which we found to be one of the strongest Lewis acids known up to date and which showed promising reactivities for activating carbon-halogen bonds.[1] This bifunctional Lewis acid-base compounds allow the formation of new polymer material.

1. Ben Saida, A., Chardon, A., Osi, A., Tumanow, N., Wouters, J., Adjieufack, A., Champagne, B., Berionni, G. *Angew. Chem. Int. Ed.*, **2019**, 58, 16889.

P12. Fluorescent Lewis Adducts: A Practical Guide to Relative Lewis Acidity

Jordan Bentley
York University, Toronto, Canada
Graduate Student
Advisor(s): Christopher Caputo

https://twitter.com/BoronBentley
@BoronBentley

Recently, we developed a new fluorescence-based method to evaluate the acidity of a series of Lewis acids across the p- and d-blocks of the periodic table with great precision. We have now considerably expanded the scope of the Fluorescent Lewis Adduct (FLA) method by systematically investigating the strength of over 50 Lewis acids in toluene; some of which have never been experimentally measured before.

(1) Gaffen, J. R.; Bentley, J. N.; Torres, L. C.; Chu, C.; Baumgartner, T.; Caputo, C. B. *Chem.* **2019**, 5, 1567-1583.

P13. Triple Decker Sandwich Complexes Containing Six Membered Ring

Moulika Bhattacharyya
University of Windsor, Windsor, ON, Canada, Canada
Post-doctoral Fellow
Advisor(s): Sundar Ghosh

https://twitter.com/bhatt_mou
@bhatt_mou

Compounds containing flat ring made of boron are very rare and only a handful of such compounds are known. Recently, we have isolated various triple-decker sandwich complexes containing puckered to flat middle rings composed of boron and non-boron elements. The complexes show 22-24-valence electrons that represent the lowest electron count triple-decker complexes. The key results of this work will be described.

[1] (a) Greenwood, N. N. Earnshaw, A.; Chemistry of the Elements; 2nd ed.; Butterworth-Heinemann: Oxford, **1997**.
[2] (a) Grimes R. N. Carboranes, 2nd ed.; Academic Press: London, **2011** (b) Grimes, R. N. *J. Organomet. Chem.* **2013**, 747, 4.
[3] (a) Thakur, A.; Chakrahari, K. K. V.; Mondal, B.; Ghosh, S. *Inorg. Chem.* **2013**, 52, 2262; (b) Mondal, B.; Mondal, B.; Pal, K.; Varghese, B.; Ghosh, S. *Chem. Commun.* **2015**, 51, 3828; (c) Mondal, B.; Bhattacharyya, M.; Varghese, B.; Ghosh, S. *Dalton Trans.* **2016**, 45, 10999.
[4] (a) Lauher, J. W.; Elian, M.; Summerville, R. H.; Hoffmann, R. *J. Am. Chem. Soc.* 1976, 98, 3219; (b) Jemmis, E. D.; Reddy, A. C. *J. Am. Chem. Soc.* **1990**, 112, 722. (c) Jemmis, E. D.; Reddy, A. C. *Organometallics* **1988**, 7, 1561.

P14. Synthesis and Reactivity of a Hypersilylsilylene

Milan Bisai
CSIR-NCL Pune, Pune, India
Graduate Student
Advisor(s): Dr. Sakya S. Sen

https://twitter.com/BisaiMilan
@BisaiMilan

Stabilization of an amidinatosilylene with a bulky hypersilyl substituent was realized with the preparation of $PhC(NtBu)_2Si\{Si(SiMe_3)_3\}$ in more than 90% yield. Subsequent to the synthesis of the silylene, we studied its reactivity toward Me_3NO, S, Se, and Te. Silaoxirane formation was observed when it was treated with acetone. Formation of tetraphosphilosilane was also realized by the reaction of chlorodiphenylphospine.

1. Bisai, M. K.; Swamy, V. S. V. S. N.; Das, T.; Vanka, K.; Gonnade, R. G.; Sen, S. S. *Inorg. Chem.* **2019**, 58, 10536.

P15. Investigating coordination tendencies of low valent Ti(III) and V(II)

(Abstract Retracted)

Hannah Bloomfield
University of Winnipeg, Winnipeg, Canada
Undergraduate Student
Advisor(s): Jamie Ritch

https://twitter.com/slowlydiene
@slowlydiene

Low oxidation state transition metals (Ti^{3+}/V^{2+}) are underexplored compared to more stable oxidation states (Ti^{4+}/V^{3+}). We theorized that the strong σ-donating and p-accepting ability of NHCs may render them good spectator ligands for these low valent metals. Various NHCs were reacted with $VCl_2(TMEDA)_2$ and $TiCl_3(THF)_3$ to study coordination tendencies, complemented by DFT calculations. This poster will highlight our experimental and computational efforts to identify ideal NHCs for stabilization.

P16. Synthesis of iron nitrosyl complexes with diethyldithiocarbamate ligands

Evan Bonnand
Cal State Polytechnic University, Pomona, USA
Undergraduate Student
Advisor(s): Dr. Stieber

https://twitter.com/Evan_Bonnand
@Evan_Bonnand

Literature reports the formation of an iron nitrosyl complex first, followed by the coordination of two dtc ligands. This work explores that approach by varying stoichiometric ratios and types of reagents used with the goal of optimizing reaction conditions and establishing an air-stable synthetic method. Deviations from literature include using Fe(III) instead of Fe(II) with both silver and sodium dtc salts. IR and NMR spectroscopy were utilized to verify the formation of the complex.

(1) Additional Materials for the Iron Nitrosyl experiment http://www.chem.ucla.edu/~bacher/CHEM174/hints/Iron_Nitrosyl.html (accessed Jun 30, **2020**).
(2) Iron Nitrosyl compounds www.chem.ucla.edu/~bacher/CHEM174/Lectures/...Nitrosyl.pptx (accessed Jun 30, **2020**).

P17. The Phospha-Bora-Wittig Reaction

Andryj Borys
University of Edinburgh, Edinburgh, Scotland
Post-doctoral Fellow
Advisor(s): Dr Michael Cowley

https://twitter.com/AndryjBorys
@AndryjBorys

Transient phosphaborenes, [$Mes^*P{=}B\text{-}NR_2$], undergo a [2+2] cycloaddition with aldehydes and ketones to give 1,2,3-phosphaboraoxetanes, which can be converted into phosphaalkenes using sub-stoichiometric N-heterocyclic carbene or $AlBr_3$, with loss of [$R_2N\text{-}BO$]$_3$. In contrast, phosphaalkenes are directly prepared from esters and amides, offering a versatile method for transforming carbonyl compounds into phosphaalkenes via the ‘phospha-bora Wittig’ reaction.

P18. Birch Bark-Oil (Maskwiomin): Synthesis and Analysis of an L'nu Indigenous Skin Ointment

Sarah Boudreau
Cape Breton University, Sydney, Canada
Undergraduate Student
Advisor(s): Dr. Matthias Bierenstiel

https://twitter.com/BoudreauChem
@BoudreauChem

Maskwiomin (birch bark-oil) is an almost forgotten L’nu medicine for the topical treatment of skin conditions (psoriasis, eczema, rashes). The L’nu method of producing the oil involves torrefaction in a campfire using a can-over-can process. The Bierenstiel group has been developing a process to control the conditions of this process with an electrical and temperature-controlled reactor. The goal of this project is to modify the conditions of the reactor to obtain better, reproducible results.

1. Flechter, O. B.; et al. *Pharm. Chem. J.* **2005**, 39, 401-404.
2. Jager, S.; et al. *Molecules* **2008**, 13, 3224-3235.
3. Krasutsky, P. A. *Nat. Prod. Rep*. **2006**, 23, 919-942.

P19. New Chemistry of Copper Halides: Alkyl C-H Fluorination and N/O/S-Nitrosation

<u>Jamey Bower</u>
The Ohio State University, Columbus, United States of America
Graduate Student
Advisor(s): Shiyu Zhang

https://twitter.com/notJamey
@notJamey

New copper halide complexes are presented that perform alkyl C-H fluorination and N/O/S-nitrosation enabled by highly covalent metal-ligand interactions. The complexes are best described as copper(II) antiferromagnetically coupled to a ligand-centered radical, which provides key insights into their reactivity. Together, these studies highlight the synergy between multireference electronic structures and ligand-centered radical reactivity of copper complexes with ambiguous oxidation states.

1. Bower, J. K.; Cypcar, A. D.; Henriquez, B.; Stieber, S. C. E.; Zhang, S. *J. Am. Chem. Soc.* **2020**, 142, 8514.
2. Bower, J. K.; Sokolov, A. Yu.; Zhang, S. *Angew. Chem. Int. Ed.* **2019**, 58, 10225.

P20. Self-assembly of nanoparticles in emulsion: a green approach to produce functional silica composites

David Brossault
University of Cambridge, Cambridge, United Kingdom
Graduate Student
Advisor(s): Prof. Alex F. Routh

https://twitter.com/BrossaultDavid
@BrossaultDavid

Silica composites are promising materials, used for biological and environmental applications. However, their preparation is often time-consuming and requires toxic chemicals or high temperatures. This poster presents a green approach to produce metal doped silica composites at room temperature via salt-induced assembly of nanoparticles in aqueous droplets.[1] Such a method is fast, tuneable and can easily be adapted to produce functional systems (e.g. Recoverable Photocatalytic Microbeads).[2]

1. Brossault, D.; Routh, A. *J. Colloid Interface Sci.* **2020**, 562, 381.
2. Brossault, D.; McCoy, T.; Routh, A. *Manuscript under review*

P21. Nanocomposites and their recent advancements

Pavan C.
Acharya and BM Reddy College of Pharmacy, Bangalore, India
Undergraduate Student
Advisor(s): Madhavi BLR

https://mobile.twitter.com/pavan_1998
@pavan_1998

Nanocomposites are versatile in their applications such as anti-corrosive, healing of bones, sensors, environmental protection, packaging, wastewater treatment, and diagnosis of tumors. Adverse effects are not just due to their individual properties of components but influence their morphology, dispersion, and interfacial characteristics. Advancements of nanocomposites are the production of flexible and rigid packaging and nanofillers creating nanocomposite structures with improved properties.

P22. A DFT and Experimental Investigation of the Ring Stability of Thionylphosphazenes

Rachele Carafa
Ryerson University, Toronto, Canada
Graduate Student
Advisor(s): Daniel Foucher & Andrew McWilliams

https://twitter.com/rachcara23
@rachcara23

Thionylphosphazenes have been shown to undergo ring-opening polymerization (ROP) at both elevated temperatures in the melt and at ambient temperatures in the presence of Lewis acids, but the mechanism on how this works is not fully understood. This study aims to apply novel DFT calculations to thionylphosphazenes and some of its derivatives to update current literature calculations while also providing more insight into their ring stability and the ROP mechanism.

McWilliams, A. R.; Gates, D. P.; Edwards, M.; Liable-sands, L. M.; Guzei, I.; Rheingold, A. L.; Manners, I.; April, R. V. *J. Am. Chem. Soc.* **2000**, 122 (6), 8848-8855.

P23. Unlocking the catalytic potential of tris(3,4,5-trifluorophenyl)borane using microwave irradiation

Jamie Carden
Cardiff University, Cardiff, United Kingdom
Graduate Student
Advisor(s): Dr Rebecca Melen

https://twitter.com/jamie_carden
jamie_carden

In this work we explore the catalytic properties of tris(3,4,5-trifluorophenyl)borane towards hydroboration, and the use of microwave irradiation to allow conventionally difficult hydroboration reactions to occur.

Carden J. L, Gierlichs L. J., Wass D. F., Browne D. L., and Melen R. L., *Chem. Comm.*, **2019**, 55, 318.

P24. Ligand Field Inversion in Sterically Confined Copper Architectures

Kurtis Carsch
Harvard University, Somerville, United States
Graduate Student
Advisor(s): Theodore A. Betley

https://twitter.com/kcarsch
@kcarsch

The isolation and characterization of formally high-valent Cu(III) complexes permits a rigorous disambiguation of electronic structure. We demonstrate ligand field inversion is general in which a physical $3d^8$ electronic configuration is inaccessible and metal-ligand multiple bonding is attenuated. These findings facilitate refined considerations of how the absence of metal-ligand multiple bonds in late transition metal complexes dictate electronic structure and multi-electron catalysis.

1. Carsch, K.M.; DiMucci, I.M.; Iovan, D.A.; Li, A.; Zheng, S.-L.; Titus, C.J.; Lee, S.J.; Irwin, K.D.; Nordlund, D.; Lancaster, K.M.; Betley, T.A. *Science* **2019**, 365, 1138.
2.Carsch, K. M.; Lukens, J. T.; DiMucci, I. M.; Iovan, D. A.; Zheng, S.-L.; Lancaster, K. M.; Betley, T. A. *J. Am. Chem. Soc.***2020**, 142, 2264.
3. DiMucci, I.M.; Lukens, J.T.; Chatterjee, S.; Carsch, K.M.; Titus, C.J.; Lee, S.J.; Nordlund, D.; Betley, T.A.; MacMillan, S.N.; Lancaster, K.M. *J. Am. Chem. Soc.* **2019**, 141, 18508.

P25. Bis-Ferrocenyl-Pyridinediimine Trinuclear Mixed-Valent Complexes with Metal-Binding Dependent Electronic Coupling

Cole Carter
Northwestern University, Evanston, United States
Graduate Student
Advisor(s): Tobin Marks

https://twitter.com/coal_carter
coal_carter

A family of ferrocene substituted Pyridinediimine metal dichloride (Fc$_2$PDI)MCl$_2$ complexes were synthesized and electronically characterized. While the parent Fc$_2$PDI ligand does not demonstrate electronic coupling between Fc units, metallation with MCl$_2$ ions promotes electronic coupling and delocalization between metals in their mixed valent state. DFT, crystallography, and spectroelectrochemistry aid in gaining granular detail about structural and electronic changes in mixed valent species.

P26. One ligand, two approach

Miguel Chacon Teran
Universidad Simon Bolivar (VE) / Universität Regensburg (DE), Caracas, Venezuela
Graduate Student
Advisor(s): Dr. Rafael Rodriguez Lugo / Dr. Robert Wolf

https://twitter.com/mchacon233
@mchacon233

Recent findings motivate to look forward P(OQuin)$_3$-chemistry.[1] In these sense, two new different P(OQuin)$_3$-approach toward second row-TM are presented. A P(OQuin)$_3$-Ru system, is a suitable catalyst for the dehydrogenative homo-/heterocoupling of silanes providing a TOF of 6000 h^{-1}. While a P(OQuin)$_3$-Rh system provide an excellent regiocontrol over the dearomative hydroboration of Py and Quin to yield 1,2-dehydroheterocycles under mild condition where additive or base are not required.

[1] (a) Rodriguez-Lugo, R. E.; Chacon-Teran, M. A.; De Leon, S.; Vogt, M.; Rosen-thal, A. J.; Landaeta, V. R., *Dalton Trans.*, **2018**, 47, 2061. (b) Chacon-Teran; M. A.; Rodriguez-Lugo, R. E.; Wolf, R.; Landaeta. V. R., Eur. J. *Inorg. Chem.* **2019**, 39-40, 4336.

P27. Synthesis of Pentasubstituted 2-Aryl Pyrroles from Boryl and Stannyl Alkynes via One-Pot Sequential Ti-Catalyzed [2+2+1] Pyrrole Synthesis/Cross Coupling Reactions

Yukun Cheng
University of Minnesota, Minneapolis, United States
Graduate Student
Advisor(s): Ian Tonks

https://twitter.com/YukunCheng1
@YukunCheng1

Pyrroles are commonly found in bioactive small molecule scaffolds, yet the synthesis of highly-substituted pyrrole cores remains challenging. Herein, we report a catalytic synthesis of 2-(9-BBN or SnR_3) pyrroles via Ti-catalyzed [2+2+1] heterocoupling of heteroatom-substituted alkynes. The resulting 2-boryl substituted pyrroles can be used in Suzuki reactions in a one-pot fashion, resulting in pentasubstituted 2-aryl pyrroles that are inaccessible via previous [2+2+1] heterocoupling strategies.

P28. Hydrostibination of acetylenes: a mechanism

Saurabh Chitnis
Dalhousie University, Halifax, Canada
Academia - Faculty/Staff
Advisor(s):

https://twitter.com/chitnislab
@chitnislab

Boranes have a low-energy vacant p-orbital and a hydridic B-H bond. This unlocks hydroboration. We have reported stibines, R_2SbH, having a low-energy σ^* LUMO and hydridic Sb-H bonds, which perform hydrostibination.[1] This poster describes experiments to discover the mechanism of this reaction.

[1] Marczenko, K. M.; Zurakowski, J. A.; Bamford, K. L.; MacMillan, J. W. M.; Chitnis, S. S. *Angew. Chem. Int. Ed.*, **2019**, 58, 18096.

P29. Cobalt PCP Carbene Complexes for the Activation of Small Molecules

Marissa Clapson
University of Calgary, Calgary, Canada
Graduate Student
Advisor(s): Dr. Warren E. Piers

https://twitter.com/Chemrissa
@Chemrissa

Co(I)-X (X = Cl or Br) PCP carbene complexes can be readily synthesized following treatment of the corresponding tetrahedral Co(II)X_2 complexes with NaHBEt_3 and Gomberg’s dimer. Treatment of the Co(I)-X complexes with either CsOH or LiCH_2TMS, results in the formation of the Co(I)-OH and Co(I)-CH_2TMS complexes, respectively. Co(I)-OH, when placed under vacuum, forms a Co(I)-O-Co(I) μ-oxo complex. Exposure of Co(I)-O-Co(I) to CO_2 results in the rapid formation of a bridging carboxylate species.

(1) Smith, J. D.; Chih, E.; Piers, W. E.; Spasyuk, D. M. *Polyhedron* **2018**, 155, 281.
(2) LaPierre, E. A.; Piers, W. E.; Gendy, C. *Organometallics* **2018**, 37 (20), 3394.
(3) Sung, S.; Wang, Q.; Kraemer, T.; Young, R. D. *Chem. Sci.* **2018**.
(4) Burford, R. J.; Piers, W. E.; Ess, D. H.; Parvez, M. *J. Am. Chem. Soc.* **2014**, 136 (8), 3256.

P30. Diverse Structure and Reactivity of Pentamethylcyclopentadienyl Antimony (III) Cations

Omar Coughlin
Nottingham Trent University, Nottingham, United Kingdom
Graduate Student
Advisor(s): Sophie Benjamin

https://twitter.com/coughlinomar
@CoughlinOmar

Heavy Group 15 organometallic complexes are emerging as powerful reagents with the potential to perform specific stoichiometric and catalytic transformations.[1-3] Harnessing advances in novel synthetic strategies and inspired by recent reports of main group cations with metallocene structures,[4-5] we have synthesised a range of pentamethylcyclopentadienyl antimony(III) cations and probed their diverse structure and reactivity.[6]

[1] Planas, O.; Wang, F.; Leutzsch, M.; Cornella, J. *Science*. **2020**, 367, 313.
[2] Stephan, D. W.; Erker, G. *Angew. Chem., Int. Ed.* **2015**, 54, 6400.
[3] Pan, B.; Gabbai, F. P. Angew. Chem., Int. Ed. *J. Am. Chem. Soc.* **2014**, 136, 9564.
[4] Zhou, J.; L. Liu, L.; L. Cao, L.; W. Stephan, D. *Chem.* **2018**, 4, 2699.
[5] N. Jones, J.; H. Cowley. A; L. B. Macdonald, C. *Chem. Commun.* **2002**, 1520.
[6] Coughlin, O.; Krämer, T.; Benjamin, S.L. *Dalton Trans.* **2020**, 49, 1726.

P31. Synthesis and Characterization of Flexible and Rigid Stannane Intermediates & Tin Polymers

Gloria D'Amaral
Ryerson University, Toronto, Canada
Graduate Student
Advisor(s): Dr. Daniel Foucher

https://twitter.com/gloriadamaral
@gloriadamaral

Polystannanes are a unique class of polymers that consist of a backbone of covalently linked tin atoms, however they display an extreme sensitivity to light and moisture. Recently, the Foucher group has demonstrated significant stability improvements when there is an increase in electron density around the tin center via hypercoordination. Using this evidence, my project focuses on synthesizing light and moisture stable polystannanes and exploring their semiconductive properties.

1. Pau, J.; D’Amaral, G. M.; Lough, A. J.; Wylie, R. S.; Foucher, D. A. *Chem. Eur. J.* **2018**, 24, 18762-18771.

P32. Mononuclear and pseudo-dinuclear Dy(III) single-molecule magnets in an “ON-OFF” state

Cody Daneluik
Brock University, Niagara Falls, Canada
Undergraduate Student
Advisor(s): Melanie Pilkington & Theocharis Stamatatos

https://twitter.com/CodyDaneluik
@CodyDaneluik

A new hexa-nucleating N_3O_3 organic chelate (L_3-) was synthesized and used for the preparation of low-coordinate, mononuclear Dy(III) single-molecule magnets (SMMs). Our first attempts led to the crystallization and structural elucidation of the 7-coordinate compound [DyL(H_2O)], which is singly H-bonded to its neighbouring monomers, yielding isolated pseudodimers that are well-separated from one another. The H-bonded dimers show interesting magnetic dynamics mainly due to exchange-bias phenomena from the communication between the two spin systems. Chemical reactivity studies have allowed us to alter the magnetic properties of these H-bonded species through the synthesis of the non-SMM complex [DyL(THF)]. Details of synthetic aspects and rationale beyond preparation of these complexes, as well as their complete magnetic characterization, will be reported in this presentation.

P33. Hydroaminoalkylation with aliphatic amines enabled by the mechanistic investigation of cyclic N,O-chelating ureate tantalum catalysts

Pargol Daneshmandkashani
University of British Columbia, Vancouver, Canada
Post-doctoral Fellow
Advisor(s): Prof. Laurel Schafer

https://twitter.com/pargol_d
@Pargol_D

The first optimized N,O-chelated cyclic ureate tantalum catalyst can be used for the hydroaminoalkylation of 1-octene with challenging N-alkyl secondary amine substrates. This catalyst offers turnover frequencies of up to 60 h^{-1} and short reaction times of approximately 1 hour. Kinetic isotope effect (KIE) studies reveal that catalytic turnover is the limiting step. Mechanistic studies show that catalytic turnover is promoted by electron rich amine substrates (Hammett plot).

P34. Towards the Preparation of Azide-Modified Silver Chalcogenolate Nanoclusters

Johanna de Jong
Western University, London, Canada
Undergraduate Student
Advisor(s): Dr. Mark Workentin, Dr. John F. Corrigan

https://twitter.com/JohdeJ
@JohdeJ

Ag nanoclusters (NCs) have applications in optical imaging, chemical sensing, and catalysis, but their ability to undergo interfacial surface chemistry is currently limited by the inertness of their organic ligands. Here we discuss progress towards functionalizing a Ag chalcogenolate NC with an azide capable of a biorthogonal click reaction: the Strain-Promoted Alkyne-Azide Cycloaddition. The ability to link molecules to the surface of NCs enables their properties to be tuned and enhanced.

35. Structure-Activity Relationships in Cationic and Neutral Indium Complexes for Ring-Opening Polymerization Reactions

Carlos Diaz
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Parisa Mehrkhodavandi

https://twitter.com/_cdlz_
@_cdlz_

Herein, we present different cationic indium with different side-arm donor groups and evaluate their effects on polymerization rates of cyclic ethers. Similarly, neutral complexes are evaluated for the ROP of cyclic esters and copolymerization of epoxides with carbon dioxide. Structure-function studies were conducted to better understand the different mechanisms involved and potentially improve the reactivity and control over the polymerizations

P36. The $Fe_2(NO)_2$ Diamond Core: A Unique Structural Motif In Non-Heme Iron-NO Chemistry

Hai Dong
University of Michigan, Ann Arbor, United States
Graduate Student
Advisor(s): Nicolai Lehnert

https://twitter.com/haidong1301
@haidong1301

Many hs-$\{FeNO\}_8$ complexes disproportionate by forming dinitrosyl iron complexes (DNICs). However, the mechanism of this reaction is not understood. The hs-$\{FeNO\}_7$ complex, [Fe(TPA)(NO)(OTf)](OTf) (1) was synthesized and characterized by different spectroscopic methods and X-ray crystallography. Upon reduction of 1 with 1 eq. of $CoCp_2$ we isolated and structurally characterized a novel dimer, $[Fe_2(TPA)_2(NO)_2](OTf)_2$, which we propose to be a potential intermediate of DNIC formation.

Dong, H. T.; Speelman, A. L.; Kozemchak, C. E.; Sil, D.; Krebs, C.; Lehnert, N. *Angew. Chem. Int. Ed.* **2019**, 58, 17695-17699.

P37. Synthesis and Structures of Anionic Rhenium Polyhydride Complexes of Boron-Hydride Ligands and their Application in Catalysis

Liam Donnelly
University of Edinburgh, Edinburgh, United Kingdom
Graduate Student
Advisor(s): Prof. Jason Love and Dr Stephen Thomas

https://twitter.com/LiamDonChem
@LiamDonChem

The rhenium complex, $[K(DME)(18\text{-}c\text{-}6)][ReH_7(BPin)_3]$ comprising hydride and boron ligands only, has been synthesized by exhaustive deoxygenation of the perrhenate anion (ReO_4-) with pinacol borane (HBPin). The structure of this complex was analysed by X-ray crystallography, NMR spectroscopy, and DFT calculations. This complex is a catalyst for the hydroboration of pyridines under simple operating procedures and is also a reagent for the C-H borylation of toluene.

Donnelly, L. J.; Parsons, S.; Morrison, C. A.; Thomas, S. P.; Love, J. B. *Submitted*

P38. Activation of a Mn(II)Mn(III)-Peroxide with Relevance to the Catalytic Cycle of Class Ib RNRs

Lorna Doyle
Trinity College Dublin, Dublin, Ireland
Graduate Student
Advisor(s): Aidan R. McDonald

https://twitter.com/ChemLorna
@ChemLorna

Ribonucleotide reductase enzymes (RNR) convert ribonucleotides to deoxyribonucleotides.[1] The biomimetic complex, $[\mathrm{Mn(II)}_2\mathrm{(BPMP)(OAc)}_2](\mathrm{ClO}_4)$ (1) reacts with superoxide, the RNR oxidising agent, to form an Mn(II)Mn(III)-peroxide which reacts with acids to form an Mn(III)Mn(IV) species. mimicking the cycle of RNR and suggests the role acid activation in the cycle of RNRs.[2],[3]

[1] Cotruvo, J. A.; Stubbe, J. *Annu. Rev. Biochem.* **2011**, 80 (1), 733.
[2] Cotruvo, J. A.; Stich, T. A.; Britt, R. D.; Stubbe, J. *J. Am. Chem. Soc.* **2013**, 135 (10), 4027. [3] (a) Suzuki, M.; Mikuriya, M.; Murata, S.; Uehara, A.; Oshio, H.; Kida, S.; Saito, K. *Bull. Chem. Soc. Jpn.* **1987**, 60 (12), 4305 (b) Blanchard, S.; Blondin, G.; RiviÃ¨re, E.; Nierlich, M.; Girerd, J.-J. *Inorg. Chem.* **2007**, 42 (15), 4568.

P39. All-solution-processed organic light-emitting diodes based on a novel and versatile benzothiazole-salophen derivative

Luis Duarte
University of Campinas, Campinas, Brazil
Post-doctoral Fellow
Advisor(s):

https://twitter.com/lgalvesduarte
@lgalvesduarte

The N,N’-bis(salicylidene)-(2-(3’,4’-diaminophenyl)benzothiazole (BTS), that undergoes Excited State Intramolecular Proton Transfer process (ESIPT) was synthesized and characterized as a strategy to construct fluorescence emission covering the entire visible spectrum. BTS was studied by steady-state and time-resolved spectroscopies. Its ESIPT balance and Zn coordination compound allowed the production of all-solution processed WOLEDs in host-guest composites.

P40. Octaboraneyl Complexes of Nickel: Monomers for Redox-Active Coordination Polymers

Maeve Dufour
University of Windsor, Windsor, Canada
Undergraduate Student
Advisor(s): Marcus Drover

https://twitter.com/maevedufour_11
@maevedufour_11

We establish the preparation, characterization, and reactivity of 1,2-bis(di(3-dicyclohexylboraneyl)propylphosphino)-ethane($P_2B^{Cy}{}_4$). The coordination of $P_2B^{Cy}{}_4$ with nickel, results in $Ni(P_2B^{Cy}{}_4)_2$ and is reactive with Lewis bases. Addition of 4,4’-bipyridine, creates an air-sensitive coordination polymer. Characterized by solid-state NMR and EPR, a charge transfer polymer was identified from an intramolecular Ni→4,4’-bpy ET, providing oxidized nickel sites and reduced 4,4’-bpy radical anion sites.

Drover, M. W.; Dufour, M.C.; Lesperance-Nantau, L.A.; Noriega, R.P.; Levin, K.; Schurko, R.W. *Chem. -Eur. J.* **2020**, DOI: 10.1002/chem.202001218

P41. Efficient Catalytic Hydrogenolysis of Halosilanes to Hydrosilanes Using an Iridium Pincer Complex and Superbases

Gabriel Durin
French Alternative Energies and Atomic Energy Commission, Paris, France
Graduate Student
Advisor(s): Thibault Cantat

https://twitter.com/DurinGabriel
@DurinGabriel

Hydrosilanes are convenient reductants but are produced via energy intensive processes[3] and generate, after use, silicon oxides wastes such as siloxanes, which are difficult to recycle. These limitations call for the development of catalytic processes able to transform Si-O bonds in siloxanes into Si-H hydrides. Previous reports4 have shown that chlorosilanes can be prepared from siloxanes. We report here an efficient hydrogenolysis of chlorosilanes (up to 79 %) using $[(^{t}BuPOCOP)IrHCl]$ complex.

1. Monsigny, L.; Feghali, E.; Berthet, J. C.; Cantat, T. *Green Chem.*, **2018**, 20, 1981.
2. Riduan, S. N.; Zhang, Y.; Ying, J. Y. *Angew. Chem. Int. Ed.*, **2009**, 48, 3322.
3. Kalchauer, W.; Pachaly, B. In Handbook of Heterogeneous Catalysis.Wiley, **2008**, 2635-2647.
4. (a) Di Giorgio, P. A.; Strong, W. A.; Sommer, L. H.; Whitmore, F. C. *J. Am. Chem. Soc*, **1946**, 68, 1380 (b) Bailey, D. L.; Sommer, L. H.; Whitmore, F. C. *J. Am. Chem. Soc*, **1948**, 70, 435-436 (c) Masaoka, S.; Bannoa, T.; Ishikawa, M. *J. Organomet. Chem.*, **2006**, 691, 174-181 (d) Roberts, J. M.; Eldred, D. V.; Katsoulis, D. E. Ind. Eng. Chem. Res., **2016**, 55, 1813-1818.
5. (a) Tsushima, D.; Igarashi, M.; Sato, K.; Shimada, S. *Chem. Lett.*, **2017**, 46, 1532-1534. See also hydrogenolysis of chlorosilanes in the presence of additives (NaI, $NaBAr_4^F$) : (b) Beppu, T.; Sakamoto, K.; Nakajima, Y.; Matsumoto, K.; Sato, K.; Shimada, S. *J. Org. Chem.*, **2018**, 869, 75-80. (c) Gluer, A.; Schweizer, J. I.; Karaca, U. S.; Wuertele, C.; Diefenbach, M.; Holthausen, M. C.; Schneider, S. *Inorg. Chem.*, **2018**, 57, 13822-13828.

P42. A Direct Comparison of Thiolate vs. Amido Donors for Bifunctional Catalysis with Mn and Cu Catalysts

Matthew Elsby
University of Ottawa, Ottawa, Canada
Graduate Student
Advisor(s): Prof. R. Tom Baker

https://twitter.com/matthew_elsby
@matthew_elsby

Base-metal complexes that utilize metal-ligand-cooperativity are highly sought. Two new Cu-SNS complexes were synthesized to compare the activity of an amido vs a thiolate donor in outer-sphere carbonyl reactivity mechanistic studies involving a “forced” outer-sphere mechanism led to the design of Mn catalysts. Insight into the Mn oxidation state in the active species in outer-sphere carbonyl reductions employing Mn(II) precatalysts are discussed.

T. Higashi, S. Kusumoto, and K. Nozaki, Cleavage of Si-H, B-H, and C-H Bonds by Metal-Ligand Cooperation, *Chem. Rev.* **2019**, 119, 10393-10402. DOI: 10.1021/acs.chemrev.9b00262

P43. Solvent-free mechanochemical synthesis of ultrasmall nickel phosphide nanoparticles and their use as catalysts for the hydrogen evolution reaction

Blaine Fiss
McGill University, Montreal, Canada
Graduate Student
Advisor(s): Dr. Audrey Moores and Dr. Tomislav Friščić

https://twitter.com/Canuk_Chemist
@Canuk_Chemist

We demonstrate the mechanochemical application of sodium phosphide as an excellent solid-state phosphorus source for the synthesis of Ni_2P nanoparticles below 3 nm in diameter, the smallest seen for the mechanochemical synthesis of metal phosphides. These nanoparticles, supported on g-C_3N_4, were successful for the hydrogen evolution reaction, generating 233.9 μmol g^{-1} h^{-1} of hydrogen, over 3 hours using broad spectrum light at room temperature, as well as being readily recyclable and reusable.

Shi, Y.; Zhang, B. *Chem. Soc. Rev.* **2016**, 45, 1529. Fiss, B. G.; Vu, N. N.; Douglas, G.; Do, T. O.; Friščić, T.; Moores, A. *Submitted*. **2020**.

P44. Vanadium Aminopyridinate Catalysts for the Reductive Coupling of Alcohols

Amanda Fogh
University of British Columbia, Vancouver, Canada
Undergraduate Student
Advisor(s): Dr.Laural Schafer

https://twitter.com/mandyfogh
@mandyfogh

The reductive coupling of alcohols is beneficial for the re-functionalization of biomass-derived material. Vanadium catalysts were investigated for this transformation. A vanadium aminopyridinate catalyst was able to perform the reductive coupling of alcohols more efficiently than previously reported catalytic systems. Many vanadium aminopyridinate complexes were synthesized towards mechanistic understanding of this catalytic system and provided insight into this underdeveloped field of study.

P45. Metal Complexes as a Promising Source for New Antimicrobials?

Angelo Frei
University of Queensland, Brisbane, Australia
Post-doctoral Fellow
Advisor(s): Dr. Mark Blaskovich

https://twitter.com/angelo_frei
@Angelo_Frei

Metal complexes are a cornerstone of medicinal chemistry, with compounds such as the anticancer drug Cisplatin still constituting one of the most important chemotherapeutics in the clinics today. However, metals have remained largely unexplored for antimicrobial applications. We have tested the antimicrobial activity of over 300,000 crowd-sourced compounds and found that metal complexes have a significantly higher hit-rate against bacteria and fungi than purely organic molecules.

Frei, A.; Zuegg, J.; Elliott, A. G.; Baker, M.; Braese, S.; Brown, C.; Chen, F.; G. Dowson, C.; Dujardin, G.; Jung, N.; King, A. P.; Mansour, A. M.; Massi, M.; Moat, J.; Mohamed, H. A.; Renfrew, A. K.; Rutledge, P. J.; Sadler, P. J.; Todd, M. H.; Willans, C. E.; Wilson, J. J.; Cooper, M. A.; Blaskovich, M. A. T., *Chem. Sci.* **2020**, 11, 2627.

P46. Ti-Mediated Intermolecular Diamination of Alkynes via [4+2]-Cycloaddition Reactions with Trapped [2+2] Intermediates

Connor Frye
University of Minnesota, Minneapolis, United States
Graduate Student
Advisor(s): Ian Tonks

https://twitter.com/ConnorFrye42
@ConnorFrye42

Accessing unsymmetrical α-diimines through acid-catalyzed condensations can be synthetically challenging. Here we report the intermolecular diamination of alkynes to afford α-diimines from Ti imidos, alkynes, nitriles, and C-nitrosos. This proposed to occur by the [4+2]-cycloaddition of a nitroso to the Ti and carbon of a trapped [2+2] diazatitanacyclohexadiene intermediate, followed by two subsequent cycloreversion steps to eliminate nitrile and afford the α-diimine and a Ti oxo.

P47. Triptycenyl phosphines as platform for the design of frustrated Lewis pair

Mathieu Gama
University of Namur, Namur, Belgium
Graduate Student
Advisor(s): Guillaume Berionni

https://twitter.com/GamaMathieu
@GamaMathieu

In 2008, Stephan defined FLPs as sterically hindered Lewis acids and bases that cannot form a covalent Lewis adduct because of steric repulsions.[1] In this work, the synthesis of triptycene-derived sterically hindered phosphines and their associations with reference Lewis acids systems of calibrated electrophilicities and Lewis acidities are investigated in the context of the development of new frustrated Lewis pairs.

1. D. W. Stephan, *Org. Biomol. Chem.* **2008**, 6, 1535

P48. Efficient Transfer Hydrogenation of Ketones using Methanol as Liquid Hydrogen Organic Carrier

Nidhi Garg
Ph.D.- IIT Kanpur, Delhi, India
Graduate Student
Advisor(s): Dr. Basker Sundararaju

https://twitter.com/Nidhigarg1994
@Nidhigarg1994

Instead of conventional, stoichiometric reducing agents or hazardous H_2 gas with transition metals, transfer hydrogenation of ketones with LOHC using transition metals is a viable alternative.But so far, only a few reports are there where methanol act as hydrogen source. We herein present, an efficient transfer hydrogenation of ketones by homogeneous iridium-bipyridonate system using methanol as LOHC. The methodology is efficient, practical, chemoselective with a wide array of ketones as scope.

Nielsen, M.; Alberico, E.; Baumann, W.; Drexler, H.-J.; Junge, H.; Gladiali, S.; Beller, M. *Nature* **2013**, 495, 85. Fujita, K.-I.; Kawahara, R.; Aikawa, T.; Yamaguchi, R. *Angew. Chem. Int. Ed.* **2015**, 54, 9057. Campos, J.; Sharninghausen, L. S.; Manas, M. G.; Crabtree, R. H. *Inorg. Chem.* **2015**, 54, 5079.

P49. Unlocking the catalytic potential of tris(3,4,5-trifluorophenyl)borane using microwave irradiation

Lukas Gierlichs
Cardiff University, Cardiff, United Kingdom
Graduate Student
Advisor(s): Rebecca Melen

https://twitter.com/LGierlichs
@LGierlichs

Enabling technology is rarely employed in main group catalysis. In this work microwave irradiation was used to enhance the reactivity of tris(3,4,5-trifluorophenyl)borane in the hydroboration of unsaturated substrates.

1. J. R. Lawson and R. L. Melen, *Inorg. Chem.*, **2017**, 56, 8627-8643.
2. J. L Carden, A. Dasgupta, and R. L. Melen, *Chem. Soc. Rev.*, **2020**, 49, 1706-1725.
3. Q. Yin, Y. Soltani, R. L. Melen and M. Oestreich, *Organometallics*, **2017**, 36, 2381-2384.
4. C. O. Kappe, *Angew. Chem. Int. Ed.*, **2004**, 43, 6250-6284.
5. J. L Carden, L. J. Gierlichs, D. F. Wass, D. L. Browne, and R. L. Melen, *Chem. Comm.*, **2019**, 55, 318-321.Â

P50. The Metalation of Neuronal Peptides with Cu(II)/(I) Modulates the Formation of Reactive Oxygen Species

Camilla Golec
Trent University, Peterborough, Canada
Undergraduate Student
Advisor(s): Dr. Sanela Martic

https://twitter.com/camillagolec
@camillagolec

Tau protein aggregation has been linked to the pathogenesis of Alzheimer’s disease (AD). However, the relationship between metal ions and the protein has not been characterized. Biologically relevant metal ions contribute to normal cellular function, but dyshomeostasis and the formation of reactive oxygen species (ROS) can lead to diseases(1-2). Several spectroscopic methods were used to study the role of Cu(II)/(I) on the formation of ROS in the presence of brain-related tau peptides.

1. Faller, P.; Hureau, C. *Chem. Eur. J.* **2012**, 18, 15910. 2. Jiang, D.; Li, X.; Liu, L,; Yagnik, G.; Zhou, F.; Tabner, J.; Allsop, D. *J. Bio. Chem.* **2014**, 289, 12052.

P51. Rational Design Approach for Improved Thermomechanical Properties in DPP-based Polymers

Renée Goodman
Universoty of Windsor, Windsor, Canada
Undergraduate Student
Advisor(s): Dr. Simon Rondeau-Gagné

https://twitter.com/ReneeBGoodman
@ReneeBGoodman

Understanding the fundamental structure-mechanical property relationship for semiconducting polymers is essential for designing more flexible organic electronics and to develop rational tools for the preparation of soft conjugated polymers. Through backbone engineering, our team is investigating the effect of fused and isolated thiophene moieties incorporated to diketopyrrolopyrrole-based conjugated polymers, and the effect of side chains on the thermomechanical properties of the semiconductors.

1. S. Zhang, M. U. Ocheje, S. Luo, D. Ehlenberg, B. Appleby, D. Weller, D. Zhou, S. Rondeau-Gagné and X. Gu, *Macromol. Rapid Commun.*, **2018**, 39, 1-8
2. S. Zhang, M. U. Ocheje, L. Huang, L. Galuska, Z. Cao, S. Luo, Y. H. Cheng, D. Ehlenberg, R. B. Goodman, D. Zhou, Y. Liu, Y. C. Chiu, J. D. Azoulay, S. Rondeau-Gagné and X. Gu, *Adv. Electron. Mater.*, **2019**, 5, 1-11.

P52. Introducing Hemilability to Cationic Indium Complexes

Chatura Goonesinghe
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Parisa Mehrkhodavandi

https://twitter.com/chaturad_g
@chaturad_g

Hemilabile ligands can influence the behavior of organometallic complexes. We report a series of cationic indium complexes bearing ligands with hemilabile pendant arms. Stability and temperature behavior of these complexes are correlated to the donicity pendant groups. The presence external donors result in fluxional behavior of the hemilabile arm with de-coordination in the presence of strong donors. This behavior allows these ligands to be used for tuning reactivity cationic indium species.

(1) Goonesinghe, C.; Roshandel, H.; Diaz, C.; Jung, H.-J.; Nyamayaro, K.; Ezhova, M.; Mehrkhodavandi, P. *Chem. Sci.* **2020**, 11 (25), 6485-6491.
(2) Diaz, C.; Ebrahimi, T.; Mehrkhodavandi, P. *Chem. Commun.* **2019**, 55 (23), 3347-3350.
(3) Jung, H.-J.; Chang, C.; Yu, I.; Aluthge, D. C.; Ebrahimi, T.; Mehrkhodavandi, P. *ChemCatChem* **2018**, 10 (15), 3219-3222.

P53. High-Efficiency Blue Photoluminescence in the $Cs_2NaInCl_6$:Sb^{3+} Double Perovskite Phosphor

Matt Gray
The Ohio State University, Columbus, United States
Graduate Student
Advisor(s): Pat Woodward

https://twitter.com/Gray3311
@Gray3311

The luminescent properties of a lead-free double perovskite $Cs_2NaInCl_6$ doped with Sb^{3+} are explored. The host crystal structure is a cubic double perovskite and has rock salt ordering of Na^+ and In^{3+} ions. It is a wide bandgap compound (5.4 eV), and substitution with Sb^{3+} leads to strong absorption in the UV due to localized $5s^2 \rightarrow 5s^1 5p^1$ transitions on Sb^{3+} centers. Radiative relaxation via a 3P1 → 1S0 transition, leads to intense blue luminescence, centered at 445 nm, with a PLQY of 79%.

Gray, M. B.; Hariyani, S.; Strom, T. A.; Majher, J. D.; Brgoch, J.; Woodward, P. M. *J. Mater. Chem. C.*, **2020**, 8, 6797-6803

P54. Elucidating the Mechanism of Oxidative Addition of Alkyl Substrates to [Ni(COD)(dppf)].

Megan Greaves
University of Strathclyde, Glasgow, UK
Graduate Student
Advisor(s): David Nelson

https://twitter.com/MeganGreaves7
@megangreaves7

This work examines the kinetics of this reaction with alkyl substrates, and shows that $Ni(dppf)_2$ is the active nickel species in the reaction with alkyl halides.(1) These reactions are first order in Ni(COD)(dppf), dppf, and alkyl halide, and inverse first order in COD. The rate expression is consistent with a rapid formation of $Ni(dppf)_2$ and a subsequent irreversible reaction with alkyl halide. The experimental data is supported by DFT studies which suggest a halide abstraction mechanism.

Bajo, S.; Laidlaw, G.; Kennedy, A., R.; Sproules, S.; Nelson, D., J. *Organometallics*, **2017**, 36, 1662

P55. It’s Better with Salt: Aqueous Ring-Opening Metathesis Polymerization at Neutral pH

Marcus Grocott
University of Birmingham, Birmingham, UK
Undergraduate Student
Advisor(s): Professor Rachel O'Reilly

https://twitter.com/marcus_grocott
@marcus_grocott

At present, acidic media is required to avert catalyst decomposition during Aqueous Ring-Opening Metathesis Polymerization, limiting its scope to non-pH-sensitive substrates. However, it is found that catalyst activity and lifetime can be improved by chloride salts at neutral pH. The ability to conduct aqueous metathesis at neutral pH is expected to enable new research avenues for polymer and organic synthesis by expanding the synthetic toolbox for reactions that involve pH-sensitive substrates.

P56. Selective C-F bond Functionalization of Polyfluorocarbon Using Frustrated Lewis Pair Approach

Richa Gupta
National University of Singapore, Singapore, Singapore
Graduate Student
Advisor(s): Dr. Rowan D Young

https://twitter.com/gupta_richa1434
gupta_richa1434

We have developed a catalytic frustrated Lewis pair approach for selective C-F bond activation in polyfluoromethyl groups with phosphine bases. The resulting phosphonium salts can be functionalized via Wittig coupling, photoredox alkylation, nucleophilic transfer and hydrophosphination reactions to install diverse functional groups into the activated C-F position. This reaction allows simple access to fluoro compounds of current interest to pharmaceutical, agrochemistry, and materials sciences.

R. Gupta, D. Mandal, R. D. Young, *J. Am. Chem. Soc*, **2018**, 140, 10682.
R. Gupta, D. Mandal, A. K. Jaiswal, R. D. Young, *J. Am. Chem. Soc.* **2020**, 142, 2572.

P57. Exploring Magnetic XY Behavior in a Quasi-2D Anisotropic Triangular Lattice of Cu(II) by Functionalized Graphene

Kriti Gupta
Indian Institute of Science Education and Research (IISER), India
Graduate Student
Advisor(s): Dr. Nirmalya Ballav

https://twitter.com/2342Kriti
@2342Kriti

Botallackite (Bo) ($Cu_2(OH)_3Br$), an anisotropic triangular spin lattice is stabilized over 2D reduced graphene oxide (rGO) via simple oxidation reduction reaction. Such an anchoring led to the oriented growth of Bo crystallites in Bo-rGO system. Bo-rGO was found to be magnetically active with a Néel transition at ~8.9 K, crossing over to possible XY anisotropy at ~5 K as revealed by dc and ac susceptibility measurements -an unprecedented observation in the field assigned to an interfacial effect.

Gupta, K.; Dadwal, A.; Jha, P. K.; Jain, A.; Yusuf, S. M.; Joy, P. A.; Ballav, N. *Inorg. Chem.* **2020**, 59, 6214.

P58. Hydrosilylative Reduction of Tertiary Amides to Amines Catalyzed by N-(Phosphinoaryl)anilido Complexes of Iron and Cobalt

Dylan Hale
Dalhousie University, Halifax, Canada
Graduate Student
Advisor(s): Dr. Laura Turculet

https://twitter.com/DylanHale1995
@DylanHale1995

The synthesis and characterization of low-coordinate Fe(II) and Co(II) complexes supported by the monoanionic P,N-ligand N-(2-dicyclohexylphosphinophenyl)-2,6-diisopropylanilide are described. Three-coordinate (P,N)Fe-hexamethyldisilazide complex (2), and four-coordinate (P,N)Fe-(3-Fe) and (P,N)Co-alkyl (3-Co) complexes were evaluated as pre-catalysts for the hydrosilylative reduction of amides with $PhSiH_3$ (5 mol% pre-catalyst, 1 equiv. $PhSiH_3$, 80°C, 1-24 h).

P59. The Synthesis of Boron-Nitrogen Doped Indenofluorenes for Organic Electronic Applications

Tyler Hannah
University of Calgary, Calgary, Canada
Undergraduate Student
Advisor(s): Warren Edward Piers

https://twitter.com/THannah77
@THannah77

This project is concerned with the synthesis of a boron-nitrogen doped indenofluorene for use as a non-fullerene acceptor in organic solar cell (OSC) applications. Previous work on this indenofluorene core was able to generate a power conversion efficiency of 2 % in an OSC device when used as an acceptor. Synthetic efforts focused on improving the device efficiency utilizing this B-N core. A synthetic pathway to the target was not able to be established, however a key intermediate was obtained.

1. Morgan, M. M.; Nazari, M.; Pickl, T.; Rautiainen, J. M.; Tuononen, H. M.; Piers, W.; Welch, G. C.; Gelfand, B. S. *Chem. Commun.* **2019**, 55, 11095-11098.

P60. Synthesis and Coordination Properties of Antimony Based Pincer Ligands

Alexander Harrison
University of Calgary, Calgary, Canada
Graduate Student
Advisor(s): Dr. Roland Roesler

https://twitter.com/aiex_harrison/
@Alex_Harrison

PCP-pincer complexes are among the most prominent representatives of their class. Comparatively, the chemistry of their heavier analogs has seen little development. Although the coordination chemistry of stibine ligands is well developed, no pincer complexes with antimony pendant donors have been reported.[1] Our investigation into these ligand platforms has yielded both surprising and expected reactivity with Rh and Ir. The synthesis and reactivity of this SbOCOSb pincer ligand will be presented.

1. Morales-Morales, D. *Mini. Rev. Org. Chem.* **2008**, 5, 141-152.

P61. Characterization of Copper Hyponitrite Complexes using X-ray Absorption Spectroscopy

Brenda Henriquez
Cal State Polytechnic University, Pomona, United States
Graduate Student
Advisor(s): Dr. Stieber

https://twitter.com/Brenda_H_2020
@Brenda_H_2020

Discrete diketiminate copper complexes formed in solution were analyzed by X-ray absorption spectroscopy. The X-ray absorption near edge structure analysis determined the oxidation state of compound 1, 2, and 4 to be +1, while compound 3 has an oxidation state of +2. The extended X-ray absorption determines coordination environment and determined compound 4 is consistent with a hyponitrite bound, suggesting one of the first examples hyponitrite complex was synthesized and isolated.

P62. Germanium Catechol Complexes: Synthesis and Assessment of their Lewis Acidity and Catalytic Activity

Andrew Henry
Western University, London, Canada
Graduate Student
Advisor(s): Kim M. Baines

https://twitter.com/andrewhenrychem
@AndrewHenryChem

Main group catalysts are currently being explored as promising alternatives to transition metal-based catalysts. While there are multiple examples of silicon Lewis acids,[1,2] germanium Lewis acid catalysts remain scarce. The synthesis of bis(catecholato)germanium complexes with two nitrogen donors has recently been reported.[3] The synthesis of a variety of germanium catechol complexes, as well as an assessment of the Lewis acidity and catalytic activity will be presented.

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3. Glavinović, M.; Krause, M.; Yang, L.; McLeod, J. A.; Liu, L.; Baines, K. M.; Friščić, T.; Lumb, J. P.; *Sci. Adv.* **2017**, 3, e1700149.

P63. CuO nanoparticles/$Ti_3C_2T_x$ MXene hybrid Nanocomposites for Detection of Toluene Gas

Angga Hermawan
Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai, Japan
Graduate Student
Advisor(s): Prof. Shu Yin

https://twitter.com/anggahermaw
@anggahermaw

We report a facile preparation of CuO/$Ti_3C_2T_x$ MXene hybrids via electrostatic self-assembly. The CuO/$Ti_3C_2T_x$ MXene exhibited the improved toluene gas sensing response (Rg/Ra) of 11.4, which is nearly 5 times higher than that of the pristine CuO nanoparticles (2.3) to 50 ppm of toluene at 250 °C. Such excellent performance showed the promising applications of metal oxides/2D hybrid materials for VOCs gas sensing.

Hermawan, A.; Zhang, B.; Taufik, A.; Asakura, Y.; Hasegawa, T.; Zhu, J.;, Shi, P.; Yin, S. *ACS Appl. Nano Mater.* **2020**, 3 (5), 4755-4766.

P64. Di-tert-butyldiphosphatetrahedrane: Catalytic Synthesis and Reactivity of the Elusive Phosphaalkyne Dimer

Gabriele Hierlmeier
University of Regensburg, Regensburg, Germany
Graduate Student
Advisor(s): Prof. Robert Wolf

https://twitter.com/ghierlmeier
@GHierlmeier

While tetrahedranes as a family are scarce, neutral heteroatomic species are all but unknown, with the only reported example being AsP_3.[1] We present the isolation of di-tert-butyldiphosphatetrahedrane, $(tBuCP)_2$, a neutral heteroatomic molecular tetrahedron which also is the long-sought-after free phosphaalkyne dimer.[2] $(tBuCP)_2$ is formed from the monomer tBuCP in a nickel-catalyzed dimerization reaction using $[(NHC)Ni(CO)_3]$ (NHC = IMes, IPr).[3]

[1] B. M. Cossairt, M.-C. Diawara, C. C. Cummins, *Science* **2009**, 323, 602.
[2] A. Chirila, R. Wolf, J. C. Slootweg, K. Lammertsma, *Coord. Chem. Rev.* **2014**, 270-271, 57.
[3] G. Hierlmeier, P. Coburger, M. Bodensteiner, R. Wolf, *Angew. Chem. Int. Ed.* **2019**, 58, 16918; Angew. Chem. **2019**, 131, 17074.

P65. Iron Complexes with N-Heterocyclic Bidentate Carbene Ligands

Alexis Hoxie
Cal State Polytechnic University, Pomona, USA
Undergraduate Student
Advisor(s): Dr. Chantal Stieber

https://twitter.com/alexis_chem
@alexis_chem

Iron complexes with bidentate N-Heterocyclic carbene ligands ($RNHC_2$; R = alkyl or aryl) have not been widely reported and have potential to be catalysts for ranges of chemical transformations. This work aims to make new Fe^0 pre-catalysts with $MesNHC_2$ ligands. $MesNHC_2$ was synthesized from mesitylimidazole, followed by addition of CH_2Br_2 to form a bis(imidazolium) salt. The salt was deprotonated with KHMDS and reacted with $FeCl_2$ to synthesize the corresponding $FeCl_2$ complex, ($MesNHC_2Me$)$FeCl_2$.

P66. Tethered tungsten-alkylidenes for the synthesis of cyclic polynorbornene via REMP: Unprecedented stereoselectivity and trapping of key intermediates

Vineet Jakhar
University of Florida, Gainesville, United States
Graduate Student
Advisor(s): Dr. Adam S. Veige

https://twitter.com/jakhar_vineet
@jakhar_vineet

This report describes an approach for preparing tethered tungsten-imido alkylidene complexes featuring a tetraanionic pincer ligand. Treating the tungsten alkylidyne [^{t}BuOCO]W≡C(^{t}Bu)(THF)$_2$ with isocyanates leads to cycloaddition occurring exclusively at the C=N bond to generate the tethered tungsten-imido alkylidenes. Unanticipated intermediates reveal themselves, including the discovery of [(O$_2$C^{t}BuC=)W((N,C)-RNCO)(THF)] and an unprecedented decarbonylation product [(tBuOCO)W(NR)(tBuCCO)].

P67. Indium-catalyzed block copolymerization of lactide and methyl methacrylate by sequential addition

Hyuk-Joon Jung
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Prof. Parisa Mehrkhodavandi

https://twitter.com/Chem_Joon
@Chem_Joon

We synthesized a series of neutral and cationic indium complexes supported by tridentate Schiff base ligands and investigated their reactivities for the homo- and block copolymerization of lactide or ε-caprolactone and methyl methacrylate by sequential addition. The block copolymers were stringently characterized by size exclusion chromatography (SEC), diffusion ordered NMR spectroscopy (DOSY), differential scanning calorimetry (DSC), and fractional precipitation techniques.

Jung, H.-J.; Yu, I.; Nyamayaro, K.; Mehrkhodavandi, P. *ACS Catal.* **2020**, 10, 6488-6496.

P68. A multistimuli responsive heteroleptic iridium(III) complex: role of hydrogen bonding in probing solvent, pH and bovine serum albumin (BSA)

Vishal Kachwal
(BITS Pilani, Pilani campus) Birla Institute of Technology, Pilani, India
Graduate Student
Advisor(s): Inamur Rahaman Laskar

https://twitter.com/kachwal_vishal
@kachwal_vishal

This article focuses on the vital role of hydrogen bonding to explain some unusual photophysical behaviors of an Aggregation-induced emission (AIE) active Iridium(III) complex. The preponderance of hydrogen bonding leads to the complex’s multifunctional character, viz., sensing ability of base and protein (BSA), pH probing, and solvatochromism. The sensitivity of the complex to BSA was measured to be 9.3 pM.

Kachwal, V., Sharma, P. K., Sarmah, A., Chowdhury, S., & Laskar, I. R, *J. Mater. Chem. C*, **2020**, 8(19), 6605-6614.

P69. Ruthenium(II) Polypyridine Complexes for Photodynamic Therapy: From In Silico Prediction to In Vivo Application

Johannes Karges
University of California, San Diego, San Diego, USA
Post-doctoral Fellow
Advisor(s):

https://twitter.com/johannes_karges
@Johannes_Karges

The currently clinically applied photosensitizers are associated with many limitations. As an alternative, the use of Ru(II) polypyridine complexes from a theoretical DFT guided search to an in-depth photophysical and biological evaluation is presented. While being able to overcome all of the limitations, the lead compound demonstrated to eradicate a drug resistant tumour inside a mouse model upon clinically relevant 1-Photon or 2-Photon excitation.

1. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao, G. Gasser, ChemRxiv **2020**, DOI: 10.26434/chemrxiv.11767995.v1
2. J. Karges, S. Kuang, Y. C. Ong, H. Chao, G. Gasser, ChemRxiv, DOI: 10.26434/chemrxiv.12440012.v1.

P70. Nuclear Medicine at War: Fighting Cancer

Jaspreet Kaur
PCTE group of Institute Ludhiana, Ludhiana, India
Academia - Faculty/Staff

Advisor(s):

https://mobile.twitter.com/cic_cheminst
@jaspree75604402

Jaspreet Kaur, Dhandeep Singh

P71. Magnesium Cobaltates: Synthesis and Reactivity

John Kelly
University of Regensburg, Regensburg, Germany
Post-doctoral Fellow
Advisor(s): Robert Wolf

https://twitter.com/jk_dude
@JK_dude

Generally, d-block metallates contain alkene or polyarene ligands and alkali metal cations, mainly lithium and potassium, yet the influence of these countercations on reactivity has been poorly explored. Our recent research has focused on d-block metallates stabilised by group 2 cations. Herein, we present the synthesis and structural characteristics of 2, the first magnesium complexes of the [Co(cod)$_2$]-anion. The reactivity and coordination chemistry of these species will be discussed.

[1] Ellis, J. E.; *Dalton Trans.*, **2019**, 48, 9538
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P72. Construction of photoresponsive coordination polymers for tuning electrical conductivity

Samim Khan
Aliah University, Kolkata, India
Post-doctoral Fellow
Advisor(s): Dr. Md. Hedayetullah Mir

https://twitter.com/samim_2k?lang=en
@samim_2k

Coordination polymers (CPs) have recently been used for the fabrication of electronic devices. A Cu(II) CP (1) has been synthesized which exhibits response with visible light enabling repetitive switching of the photocurrent displaying substantial on-off ratio. Secondly, a Cd(II) based CP (2) has been synthesized which undergoes [2+2] cycloaddition reaction to generate dimerized CP (3). Compound 2 shows better charge transport property than 3, may be due to π-π stacking interactions in 2.

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2. Islam, S.; Datta, J.; Maity, S.; Dutta, B.; Khan, S.; Ghosh, P.; Ray P. P.; Mir, M. H.; *Cryst. Growth Des*. **2019**, 19, 4057.

P73. Three-in-one is really better: exploring the sensing and adsorption properties in a newly designed metal-organic system incorporating a copper (ii) ion

Mohammad Shahnawaz Khan
Aligarh Muslim University, Aligarh, India
Graduate Student
Advisor(s): Dr Mohd Khalid

https://twitter.com/Sarcastickhan1
@Sarcastickhan1

In this work we have successfully designed a 2-D copper(II) based coordination polymer for the functional applications. Fluorescence sensing property demonstrates the high selectivity and sensitivity towards nitrobenzene and Fe^{3+}. Moreover, CP (1) acted as tremendous adsorbent material for natural dyes with different charges and size i.e. methylene blue (MB), methyl orange (MO) and rhodamine-B.

[1] Khan, M. S.; Khalid, M.; Ahmad, M. S.; Shahid, M.; & Ahmad, M. *Dalton Trans.* **2019**, 48, 12918.
[2] Nagarkar, S. S.; Joarder, B.; Chaudhari, A. K.; Mukherjee, S.; & Ghosh, S. K. Angew. Chem. **2013**, 125, 2953.

P74. Bio-derived and Biodegradable Lignin-graft-Poly(lactic acid) Copolymers

Diana Kim
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Dr. Parisa Mehrkhodavandi

https://twitter.com/Diana_Chem
@Diana_Chem

Lignin is the second most abundant bio-derived material on earth after cellulose. Nonetheless, this cheap and renewable material has been underutilized due to the complexity of its structure. In this study, we aim to functionalize lignin with controlled molecular weight and enantiopure biodegradable poly(lactic acid) (PLA). The prepared PLA is successfully grafted to lignin via graft-to synthetic strategy and a series of lignin-graft-PLA copolymers are synthesized.

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3. Kadla, J. F.; Kubo, S.; Venditti, R. A.; Gilbert, R. D.; Compere, A. L.; Griffith, W.,. *Carbon* **2002**,40 (15), 2913-2920.
4. Johansson, C.; Bras, J.; Mondragon, I.; Nechita, P.; Plackett, D.; Simon, P.; Gregor Svetec, D.; Virtanen, S.; Giacinti Baschetti, M.; Breen, C.; Aucejo, S., *Bioresources* **2012**, 7 (2), 2506-2552.
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P75. Monoanionic pincer complexes of bismuth: potential new class of Lewis acid catalysts

Marcus Kindervater
Dalhousie University, Halifax, Canada
Graduate Student
Advisor(s): Dr. Saurabh Chitnis

https://twitter.com/mbkindervater
@mbkindervater

Herein we debut the coordination chemistry of a rigid P_2N_3 phosphinimine and a flexible PNP pincer complex of bismuth that show varying degrees of planarity. We further demonstrate the ability for PNP-Bi complexes to support highly electrophilic Bi(III) centers with potential application as Lewis acid catalysts.

Kindervater, M. B.; Hynes, T.; Marczenko, K. M.; Chitnis, S. S. *Dalton Trans.* **2020**. https://doi.org/10.1039/D0DT01413C.

P76. Structural Transformations of a Mechanochemically Generated Polymorphic Organocalciate

Ross Koby
Vanderbilt University, Nashville, United States
Graduate Student
Advisor(s): Timothy P. Hanusa

https://twitter.com/rawssk0be
@rawssk0be

Ball milling K[A’] (A’ = $[1,3\text{-}(SiMe_3)_2C_3H_3]^-$) with CaI_2 yields [KCaA’], which initially forms a structure (1) likely containing sigma-bound allyl ligands. Over time, the compound rearranges to a form (2) with eta 3-bound allyl ligands, which can be crystallized as a coordination polymer. The transformation from 1 to 2 can be followed by NMR and has been modeled with DFT calculations. Form 2 is capable of initiating polymerization of methyl methacrylate and isoprene at extremely low temperature.

P77. The Rate of Cadmium Metallation of Metallothionein is Dependent on Structure and Binding Pathways

Natalie Korkola
Western University, London, Canada
Graduate Student
Advisor(s): Dr. Martin Stillman

https://twitter.com/nataliekorkola
@NatalieKorkola

The protein metallothionein (MT) binds up to 7 divalent metals using 20 cysteines.[1] Metallation proceeds by either binding to terminal cysteines or through bridging “clusters”.[2] Here, the kinetics of these cadmium metallation pathways using stopped flow combined with UV-visible spectroscopy were studied. The beaded pathway proceeded much faster than the cluster pathway. Unfolding of apo-MT also slowed down the rate.[3] This provides a further understanding of MT’s metallation pathways.

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P78. Combining Metal-Metal and Metal-Ligand Cooperativity Using a Naphthyridine-based Proton-responsive PNNP ‘Expanded pincer’

Errikos Kounalis
Utrecht University, Utrecht, The Netherlands
Graduate Student
Advisor(s): Dr. ing. D.L.J. (Danny) Broere

https://twitter.com/ErrikosKounalis
@ErrikosKounalis

Inspired by nature,[1-2] we have synthesized a proton responsive ‘expanded pincer’ ligand that can bind multiple 1st-row transition metals in close proximity and facilitate metal-metal and metal-ligand cooperativity. We have demonstrated cooperative activation of H_2 on a dicopper (I) complex, concomitant with the formation of a uniquely shaped Cu_4H_2 cluster.[3] Additionally, organocopper complexes and their remarkable structural behavior will be discussed.[4]

[1] Sippel, D.; Rohde, M.; Netzer, J.; Trncik, C.; Gies, J.; Grunau, K.; Djurdjevic, I.; Decamps, L.; Andrade, S.L.A, Einsle, O. *Science*. **2020**, 359, 6383, 1484-1489.
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[3] Kounalis, E.; Lutz, M.; Broere, D.L.J. *Chem. Eur. J.* **2019**, 25, 58, 13280-13284.
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P79. Autonomous Chemical Robot Discovers the Rules of Coordination Chemistry

Daniel Kowalski
University of Glasgow, Glasgow, UK
Graduate Student
Advisor(s): Prof Lee Cronin

https://twitter.com/dankowalskichm
@dankowalskichm

Digital chemistry is a rapidly growing discipline, although the adoption of automation has been slower in coordination chemistry than other areas.[1-3] We demonstrate the use of an unsupervised algorithm to robotically search a predefined chemical space for novel coordination complexes based on the data from in situ analysis.[4] Without any prior knowledge or simulation of chemistry, the algorithm has permitted the isolation of multiple new complexes and further in situ observations.

[1] Coley, C. W.; Eyke, N. S.; Jensen, K. F. *Angew. Chem. Int. Ed.* **2020**, 59, ASAP
[2] Gromski, P. S.; Henson, A.; Granda, J.; Cronin L. *Nat. Rev. Chem.* **2019**, 3, 119
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P80. Fused Inorganic Rings Containing Germanium and Boron Towards Hybrid Materials

Kelsie Krantz
University of Virginia, Charlottesville, United States
Graduate Student
Advisor(s): Robert J. Gilliard, Jr.

https://twitter.com/kek_kelsie
@kek_kelsie

The synthesis of highly conjugated organic molecules has advanced light emitting diodes and other electronic display technologies. By incorporating other p-block elements into organic systems, improved optoelectronic properties are achieved. This poster will highlight a new class of pyrene-fused N-heterocyclic germylenes which display extremely large twist angles. Additionally, the isolation, characterization, and photoluminescent properties of their boron analogues will also be discussed.

Krantz, K. E.; Weisflog, S. L.; Frey, N. C.; Yang, W.; Dickie, D. A.; Webster, C. E.; Gilliard, R. J. Jr., *Chem. Eur. J.* **2020**, DOI: 10.1002/chem.202002118 Krantz, K. E.; Weisflog, S. L.; Yang, W.; Dickie, D. A.; Frey, N. C.; Webster, C. E., Gilliard, R. J. Jr., *Chem. Commun.* **2019**, 55, 14954

P81. Synthesis and Characterization of Heteroleptic Redox Active Bismuth Dithiolene and Dithiolate Complexes

Viveka Kulkarni
Mount Allison University, Sackville NB, Canada
Undergraduate Student
Advisor(s): Dr. Glen Briand

https://twitter.com/KulkarniViveka
@KulkarniViveka

Redox catalysis often feature toxic transition metal centers that can be harmful to both human health and the environment. Bismuth is a potential alternative due to its relatively low toxicity and cost, but does not possess accessible oxidation states. The current study focuses on the use of redox non-innocent ligands to impart redox activity on a heteroleptic bismuth complexes. The synthesis and structural characterization of two bismuth 3,4-toluenedithiolate complexes is reported.

P82. Dinuclear Reductive Elimination of H_2 from an Ir(III)-H is Made Possible by Metal/Ligand Proton Tautomerism

Jonathan Kuo
University of Pennsylvania, Philadelphia, United States
Post-doctoral Fellow
Advisor(s): Karen Goldberg

https://twitter.com/JonathanLKuo
jonathanlkuo

We have synthesized a square-planar Ir(I) carbonyl compound bearing a protic bis-pyrazolatopyridine ligand. Additional ligands PPh_3 or ^{t}BuPy induce tautomerism, where a ligand-based proton migrates to the metal forming an octahedral Ir(III)-H. In solution, the hydride undergoes the formal dinuclear reductive elimination of H_2, generating the corresponding Ir(II) dimer. This is possible because the hydride establishes a [^{t}BuPy] dependent equilibrium with its ligand protonated Ir(I) tautomer.

P83. Heteroatom-Rich Ligands for Heavy Metal Sequestration

Jan-Willem Lamberink
Western University, London, Canada
Graduate Student
Advisor(s): Johanna Blacquiere, Paul Ragogna

https://twitter.com/JwLamberink
@JwLamberink

Contamination of generated effluent with heavy metals is an issue that plagues many industries. The phosphane-ene reaction can generate phosphorus rich networks that are promising materials for heavy metal sequestration. Modification and study of cross-linkers provides crucial insight into the effectiveness of the overall material. These studies have led to the use of an underused methodology for P-H bond addition to C=N bonds, which can be utilized in the synthesis of heteroatom-rich polymers.

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P84. Ligand-Assisted Volatilization and Thermal Stability in Mo(VI) Compounds

Michael Land
Carleton University, Ottawa, Canada
Graduate Student
Advisor(s): Sean Barry

https://twitter.com/MikeL4nd
@MikeL4nd

Herein, we investigate the volatility and thermal stability of the parent bis(tert-butylimido)dichloromolybdenum(VI) compound, and the effect of neutral ligands including amines, phosphines, ethers, and an N-heterocyclic carbene. Their volatility and thermal stability are assessed using thermogravimetric analysis and differential scanning calorimetry, respectively[1]. The compounds have also been ranked using a Figure of Merit system[2] based upon observed thermal behavior.

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P85. Solubility Measurements of Strontium Carbonate in Aqueous Ammonium Chloride for Aqueous Extraction of Strontium Carbonate from Strontium Molybdates

Andres Lara Contreras
Department of Chemistry and Chemical Engineering - Royal Military College of Canada, Kingston, Canada
Graduate Student
Advisor(s): Dr. Emily Corcoran and Dr. Jennifer Scott

https://twitter.com/AndresLaraCo
@AndresLaraCo

Sr-Mo-O compounds are synthesized to understand the thermochemistry of nuclear fuels. The formation of $SrCO_3$ can affect subsequent thermodynamic measurements. A solid-liquid $SrCO_3$ extraction method has been developed using aqueous NH_4Cl, which preserves the solid Sr-Mo-O phase intact. Given the lack of S-L equilibria data for the $SrCO_3$ + NH_4Cl + H2O system, a preliminary assessment of solubility limits in the temperature range 298 to 348 K and NH_4Cl concentration of 0.25 to 2.00 M is presented.

P86. Iron Coordination Complexes for Ultra-High Efficiency Monolayer Electrochromic Materials

Nadia Laschuk
Ontario Tech University, Oshawa, Canada
Graduate Student
Advisor(s): Dr. Olena V. Zenkina

https://twitter.com/laschuk_
@laschuk_

Terpyridine (tpy) coordinated to Fe(II) forms a coloured complex. Electrochemical oxidation from Fe(II) to Fe(III) under low potentials results in a reversible bleaching of the complex, known as electrochromic materials (ECMs). We synthesized and characterized a series of iron(II) bis(tpy) complexes, and then covalently attached them to novel conductive inorganic nanoparticle (NP) supports. Together, these created atom efficient ECMs with ultrahigh durability and high colouration efficiencies.

Laschuk, N.I.; Obua, A.; Ebralidze, I.I.; Fruehwald, H.M.; Poisson, J.; Egan, J.G.; Gaspari, F.; Naumkin, F.Y.; Easton, E.B.; Zenkina, O.V. ACS *Appl. Electron. Mater.* **2019**, 1, 1705-1717.

P87. Exploring Through-Bond and Through-Space Magnetic Communication in 1,3,2-Dithiazolyl Radical Complexes

Dominique Leckie
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Dr. Jeremy Rawson

https://twitter.com/ladominiquee
@ladominiquee

The field of single molecule magnets (SMM) has provided access to systems in which individual bits of data can be stored at the molecular (nm and sub-nm) scale. The use of paramagnetic ligands has attracted attention to increase the spin ground state in polynuclear complexes. While ligands comprising heavier p-block elements have the potential to increase magnetic anisotropy. Here, we present the characterization of prototypical complexes of the thiazyl radical MBDTA with $M(hfac)_2$.(1)

(1) Leckie, D.; Stephaniuk, N. T.; Arauzo, A.; Campo, J.; Rawson, J. M., *Chem. Commun.* **2019**, 55 (66), 9849-9852.

P88. 2-(2'-Pyridyl)-4,6-diphenylphosphinine: A Chemically Non-Innocent Ligand Toward Iron(0) and Nickel(0)

Julia Leitl
Institute of Inorganic Chemistry, University of Regensburg, Regensburg, Germany
Graduate Student
Advisor(s): Prof. Dr. Robert Wolf

https://twitter.com/julia_leitl
@julia_leitl

Phosphinines are versatile ligands for transition metals due to their special steric and electronic properties.[1] In this work, new iron(0) complexes [Cp*FeL]- (1-σ and 1-π, Cp* = C_5Me_5) containing the chelating ligand 2-(2'-pyridyl)-4,6-diphenylphosphinine (L) have been prepared and found to undergo facile reaction with CO_2 under ambient conditions.[2] In contrast, L forms of a homoleptic phosphinine complex $[Ni(L)_2]$ (4) with a Ni(0) precursor, which shows reactivity toward phenyl halides.

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P89. How Do Metal Ions Affect the Ability of a Flavonoid to Quench the Superoxide Anion Radical?

Tyra Lewis
Department of Forensic Science, Environmental and Life Sciences, Trent University, Peterborough, Canada
Undergraduate Student
Advisor(s): Dr. Sanela Martic

https://twitter.com/siwelaryt
@siwelaryt

Quercetin (QCR) is a strong antioxidant against superoxide anion radical (SAR)(1). While biologically-relevant metal ions regulate SAR, their roles on activity of QCR is not fully understood. By using electrochemical method(2), the ability of Fe(III) and Cu(II) to modulate QCR activity was measured for metal ion:QCR ratio and complex type. Data indicated that antioxidant ability of QCR was regulated by metal ion, whilst the Cu(II)-QCR complex exhibited greatest antioxidant activity with SAR.

1. Gil, E.S.; Couto, R.O. *Braz. J. Pharmacogn.* **2013**, 23 (3), 542.
2. Zabik, N.L.; Anwar, S.; Ziu, I.; Martic-Milne, S. *Electrochim. Acta.* **2019**, 296, 174.

P90. Mesoionic N-heterocyclic olefin carbene tautomerization

Qiuming Liang
University of Toronto, Toronto, Canada
Graduate Student
Advisor(s): Datong Song

https://twitter.com/WalterQLiang
@WalterQLiang

N-heterocyclic olefins (NHOs), sometimes referred to as deoxy-Breslow intermediates, have been widely studied and found broad applications in coordination chemistry and (organo)catalysis. We herein present an unprotected mesoionic N-heterocyclic olefins (mNHO) which can tautomerize into mesoionic carbenes (MIC) at room temperature. Experimental and computational studies allow us to compare their thermodynamic properties. An unusual O_2 activation will also be presented.

P91. Mechanism of 8-Aminoquinoline Directed Ni-Catalyzed C(sp^3)-H Functionalization: Unanticipated Mononuclear and Dinuclear Paramagnetic Ni(II) Species.

Jun Yang Liu
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Dr. Samuel Johnson

https://twitter.com/ljyangjun
@ljyangjun

The catalytic activation of C-H bonds using first row transition metals has been an ideal choice in constructing new C-C bonds, but first row metal such as Ni, is less reactive/selective. A common strategy is using directing groups(8-AQ). Although a wide range of Ni-catalyzed C-H activations are reported, studies probing the mechanisms remain limited. This study aims at identifying catalytically-relevant key intermediates, and describing the mechanism of directed nickel-catalyzed C-H arylation.

P92. Polymeric pH-Activated Nanoparticles for Lipo-toxic Cell Application

Kaitlynn Lopes
Boston University, Boston, United States
Graduate Student
Advisor(s):

https://twitter.com/klvettegirl715
@klvettegirl715

Non-alcoholic fatty acid liver disease (NAFLD) is characterized by cellular lipotoxicity, increased lysosomal pH, and inhibited autophagic processes. We propose the development of polymeric pH-activated nanoparticles for acid delivery to the lysosomes within lipo-toxic cells. Nanoparticles with an average diameter of approximately 100 nm and a polydispersity between 0.1 and 0.2 were deemed ideal for cellular uptake. Optimal nanoparticles were formed and determined to be non-cytotoxic.

1. Younossi, Z., Anstee, Q.M., Marietti, M, Hardy, T., Henry, L., Eslam, M., George, J., & Bugianesi, E. *Nature Reviews Gastroenterology & Hepatology.* **2018**, 15,11-20.
2. Trudeau, K.M., Colby, A.H., Zeng, J., Las, G., Feng, J.H., Grinstaff, M.W., Shirihai, O.S. *J Cell Biol.* **2016**, 214 (1), 25-34.
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P93. Tellurium-Containing Polymers for Organic Electronics

Bruno Luppi
University of Alberta, Edmonton, Canada
Graduate Student
Advisor(s): Eric Rivard

https://twitter.com/luppi_bruno
@luppi_bruno

The field of polymer electronics often relies on complex molecular/polymeric structures and metastable device architectures to achieve high-performance.[1,2] This poster describes the synthesis of structurally simple Te-containing polymers of interest for photovoltaics.[3] These show reduced band gaps (e.g. 1.3 eV) when compared to their structurally analogous polythiophenes.[4] Additionally, cycloalkyl-fused oligomers reveal a drastic band gap reduction when the cycloalkyl ring size is altered.

1. L. Dou, Y. Liu, Z. Hong, G. Li and Y. Yang, *Chem. Rev.* **2015**, 115, 12633.
2. L. Lu, T. Zheng, Q. Wu, A. M. Schneider, D. Zhao and L. Yu, *Chem. Rev.*, **2015**, 115, 12666.
3. B. T. Luppi, D. Majak, M. Gupta, E. Rivard and K. Shankar, *J. Mater. Chem. A*, **2019**, 7, 2445.
4. B. T. Luppi, R. McDonald, M. J. Ferguson, L. Sang and E. Rivard, *Chem. Commun.*, **2019**, 55, 14218.

P94. Benzene Insertion into a Nickel Hydride Bond

Casper Macaulay
Dalhousie University, Halifax, Canada
Post-doctoral Fellow
Advisor(s): Mark Stradiotto

https://twitter.com/eTheR_ealCasper
@eTheR_ealCasper

Treatment of (PN)NiNHDipp (PN = N-phosphinoamidinate ligand) with Me_2PhSiH in benzene solvent yielded the crystallographically characterized, antifacial-coordinated, dinuclear species (PN)Ni(μ^2-η^3: η^3-C_6H_8)Ni(PN) (1), representing the first isolated example of benzene insertion into a Ni-H bond. Efforts to generate (1) via β-hydride elimination of alkyl complexes instead afforded low-coordinate agostic alkyl complexes, including (PN)Ni(Neopentyl), the first neutral Ni(II) γ^3-agostic alkyl complex.

1. Macaulay, C. M.; Samolia, M.; Ferguson, M. J.; Sydora, O. L.; Ess, D. H.; Stradiotto, M.; and Turculet, L. *Dalton Trans.* **2020**, 49, 4811-4816.

P95. Synthesis of sterically hindered 9-phosphatriptycenes and computational investigation of their properties

Damien Mahaut
University of Namur, Namur, Belgium
Graduate Student
Advisor(s): Prof. G. Berionni

https://twitter.com/DMahautChem
@DMahautChem

Frustrated Lewis Pairs (FLPs) consist in bulky Lewis acid and base which cannot form a Lewis adduct because of steric repulsions and have been extensively used as transition metal-free catalysts for hydrogenations.[1] In this context, 9-phosphatriptycenes constitute promising Lewis bases due to their cage-like structures. In this poster, the synthesis of sterically hindered 9-phosphatriptycenes will be presented as well as a DFT investigation of their properties and potential for FLP chemistry.

1a. Stephan, D. W., *Science* **2016**, 354, 1248.
1b. Lam, J.; Szkop, K. M.; Mosaferi, E.; Stephan, D. W.; *Chem. Soc. Rev.* **2019**, 48, 3592.

P96. Photophysical and Optical Properties of Semiconducting Polymer Nanoparticles Prepared from Hyaluronic Acid and Polysorbate

Aleena Malik
Univeristy of Windsor, Windsor, Canada
Undergraduate Student
Advisor(s): Dr. Simon Rondeau- Gagné

https://twitter.com/amalik283
@amalik283

Diketopyrrolopyrrole-based semiconducting polymer nanoparticles prepared from hyaluronic acid and polysorbate were prepared and characterized using transmission electron microscopy, dynamic light scattering, small-angle neutron scattering, and optical spectroscopy to determine their photophysical and optical properties. These nanoparticles were found to exhibit characteristics that are similar to the native polymers and show promise for application in biomedical imaging and nanomedicine.

P97. S-S antioxidant assessment

Basel Mansour
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): James W. Gauld

https://twitter.com/BaselMa42697042
@BaselMa42697042

The assessment of the antioxidant activity of different compounds contains S-S bond by using computational methods.

P98. Bismuthanyl-Stibanes: The first neutral Bi-Sb σ-bonds

Kate Marczenko
Dalhousie University, Halifax, Canada
Graduate Student
Advisor(s): Dr. S. Chitnis

https://twitter.com/KMMarczenko
@KMMarczenko

Thermally-robust bismuthanylstibanes[1] are prepared in a one-step, high yield reaction, providing the first examples of neutral Bi-Sb σ-bonds in the solid state. DFT calculations indicate that the bis(silylamino)naphthalene scaffold is well-suited for supporting otherwise labile bonds. The reaction chemistry of the Bi-Sb bond is exploited by showing insertion of a sulfur atom, providing the first documented example of a Bi-S-Sb bonding moiety.

[1] Marczenko, K. M., Chitnis, S. S., *Chem. Commun.*, **2020**, In Press.

P99. Dendronized Side Chains in Conjugated Polymers Toward More Robust Organic Electronics

Gage Mason
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Simon Rondeau-Gagne

https://twitter.com/magegason
@magegason

Organic semiconductors are used in organic electronics due to their solution processability and optoelectronic properties. Efforts have been made to improve the mechanical properties and solubility while enhancing stability. Several methodologies have been utilized to improve these properties, but sidechain engineering remains one of the most efficient. Recently, our group has incorporated dynamic bonding moieties (ligands or hydrogen bonding) to improve the thermomechanical properties.

1. Heeger, A. J. et al. *Adv. Mater.* **2014**, 26, 2993-2998.
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3. Bazan, G. C. et al. *Angew. Chem., Int. Ed.* **2014**, 53, 14378-14381.
4. Brabec, C. J. et al. *Adv. Funct. Mater.* **2014**, 24, 1449-1457.
5. Andreasen, J. W. et al. *J. Mater. Chem. A* **2015**, 3, 17022-17031.
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P100. Synthetic Efforts Towards Biologically Active Chelated Boron Complexes

Kathleen May
Ryerson Univeristy, Toronto, Canada
Graduate Student
Advisor(s): R. A. Gossage and S. A. Westcott

https://twitter.com/khem4may
@khem4may

Boron-containing compounds have been overlooked when considering drug design. More recently popularized by the discovery of 5-fluorobenzoxaborole, boron-containing compounds have seen increased use and research interest. We intend to take advantage of the known biological activity of various azoles and use them with those a boron centre to increase biological efficacies. Ligand synthesis and advancements as well as future directions to determine their biological activity will be noted.

P101. Nickel-Catalyzed Cross-Coupling of Sulfonamides With (Hetero)aryl Chlorides

Ryan McGuire
Dalhousie University, Halifax, Canada
Graduate Student
Advisor(s): Dr. Mark STradiotto

https://twitter.com/_McGuireRyan
@_mcguireryan

The development of Ni-catalyzed C-N cross-couplings of sulfonamides with (hetero)aryl chlorides is reported. These transformations, which were previously achievable only with Pd catalysis, are enabled by use of air-stable (L)NiCl(o-tol) pre-catalysts (L=PhPAd-DalPhos and PAd_2-DalPhos), without photocatalysis. The collective scope of (pseudo)halide electrophiles demonstrated herein is unprecedented for any reported catalyst system for sulfonamide C-N cross-coupling.

McGuire, R. T.; Simon, C. M.; Yadav, A. A.; Ferguson, M. J.; Stradiotto, M. *Angew. Chem. Int. Ed.* **2020**, 59, 8952-8956.

P102. Computational Studies on the Formation of Biological Per/Polysulfides

Paul Meister
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Prof. James W. Gauld

https://twitter.com/meisterp3/
@meisterp3

Sulfur is a rare element in biology and typically exists as one of two proteinogenic amino acids, cysteine and methionine. They have important roles in redox signaling, protein folding, and enzymatic function. Persulfides (RSSH) are reactive intermediates making them a difficult topic to study. Herein, we used computational methods to study the formation of persulfide bonds and the extension of a sulfur chain within sulfide:quinone oxidoreductase (SQR) from a hyperthermoacidophilic archaea.

P103. Probing the Sequence of Copper-Thiolate Cluster Formation in Metallothionein Using Native ESI-Mass Spectrometry

Adyn Melenbacher
Western University, London
Graduate Student
Advisor(s): Professor Martin Stillman

https://twitter.com/adynmelenbacher
@adynmelenbacher

Cu is vital for life. Free cellular Cu catalyzes the formation of dangerous radicals. Cellular copper chaperones are required to avoid uncontrolled redox chemistry. Metallothionein (MT) binds Zn(II) and Cu(I). ESI-MS can be used to view the series of Cu(I)-thiolate clusters forming in MT, however it is unclear which cysteines bind to the Cu(I) first. Isolated domain fragments of MT have been used to determine domain preference of Cu(I) binding through detailed native ESI-MS studies.

Scheller, J. S.; Irvine, G. W.; Wong, D. L.; Hartwig, A.; Stillman, M. J. *Metallomics*. **2017**, 9, 447.

P104. Mechanistic Investigation of the Nickel-Catalyzed Carbonylation of Alcohols

Maximilian Menche
Catalysis Research Laboratory (CaRLa), Germany
Graduate Student
Advisor(s):

https://twitter.com/maxmenche
@maxmenche

The carbonylation of alcohols represents an atom-efficient methodology for the preparation of carboxylic acids. Current processes either rely on harsh reaction conditions or precious metals[1-2]. Here, we present a mechanistic study of a catalytic system based on NiI_2, which can regioselective carbonylate benzylic alcohols. Quantum-chemical computations were used to evaluate the underlying mechanistic processes. They revealed that two mechanisms are responsible for the observed reactivity.[3]

[1] Samel, U.; Kohler, W.; Gamer, A. O.; Keuser, U.; Yang, S.; Jin, Y.; Lin, M.; Wang, Z. Propionic acid and derivatives in Ullmann's Encyclopedia of Industrial chemistry, Wiley-VCH, Weinheim, **2014**.
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[3] Sabater, S.; Menche, M.; Ghosh, T.; Krieg, S.; Rück, K. S. L.; Paciello, R.; Schäfer, A.; Comba, P.; Hashmi, A. S. K.; Schaub, T. *Organometallics* **2020**, 39, 870-880.

P105. Exploring the photocatalytic hydrogen production by ruthenium polypyridine and cobaloxime assemblies

AB MIR
IIT Gandhinagar, Baramulla, India
Undergraduate Student
Advisor(s): Dr Armab Dutta

https://twitter.com/InorgChem
@mir_qayoom

Axial coordinated imidazole derivatives; such as imidazole carboxylic acids and histidine; directly linked an identical Co(dimethylglyoxime)$_2$ core is shown to catalyze the reduction of aqueous proton to hydrogen (H_2) in light-driven photocatalytic reactions in water near neutral pH.

P106. Sustainable Synthesis of Pyridines, Quinolines and Pyrimidines by Ru Catalyzed Acceptorless Dehydrogenation of Alcohols and C-C/C-N Coupling

Rajarshi Mondal
University of Manitoba, Winnipeg, Canada
Post-doctoral Fellow
Advisor(s): Dr. David E. Herbert

https://twitter.com/JuchemMondal
@JuchemMondal

The acceptorless dehydrogenation of widely available biomass generated alcohols followed by coupling with amines can lead to sustainable and atom economical routes to core organic building blocks including nitrogen-containing heterocycles. In this presentation, preparation of a simple novel P^N ligand based Ru catalyst for acceptorless dehydrogenation of alcohols, substrate scope for N-heterocycle synthesis such as pyridines, quinolines and photo-emissive pyrimidines will be discussed.[1]

[1]. (a) Mondal, R.; Herbert, D. E. *Organometallics* **2020**, 39, 1310 (b) Mondal, R.; Lozada, I.B.; Davis, R. L.; Williams, J. A. G.; Herbert, D.E. *Inorg. Chem.* **2018**, 57, 4966 (c) Mondal, R.; Giesbrecht, P. K.; Herbert, D. E. *Polyhedron* **2016**, 108, 156.

P107. Development of Green Solvent Processable Semiconductors for Printed Electronics

Madison Mooney
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Simon Rondeau-Gagne

https://twitter.com/Madison77772905
@Madison77772905

Our research aims to minimize the impact of electronic waste on the environment by developing a series of green solvent processable organic semiconductors for Printed Electronics. By incorporating hydrogen-bonding saccharide moieties through side-chain engineering, a series of semiconducting polymers were synthesized to be soluble in environmentally-friendly alcohol-based solvents, rather than the toxic halogenated solvents typically used for processing of these materials.

P108. A fluorine transfer reaction: C-F bond activation leading to nucleophilic fluorination

Patrick Morgan
University of Nottingham, Nottingham, United Kingdom
Graduate Student
Advisor(s): Pete Licence

https://twitter.com/azure_wanderer
@azure_wanderer

We present a first account of a transfer fluorination protocol where fluorine is transferred from a perfluorinated moiety onto a non-fluorinated substrate. The reaction occurred via the concurrent C-F bond activation, fluorine transfer, and C-F bond formation resulting in selective fluorination of an organic target. Fluorine transfer was tracked using in-situ ReactIR, where the rate of C-F bond activation was observed to match the rate of C-F bond formation.

(1) Morgan, P. J.; Hanson-Heine, M. W. D.; Thomas, H. P.; Saunders, G. C.; Marr, A. C.; Licence, P. *Organometallics* **2020**, 39 (11), 2116-2124.

P109. The Influence of Carbon Donor Ligands on Biomimetic High-Spin Iron Complexes for N_2 Reduction

Alexandra Nagelski
Yale University, New Haven, United States
Graduate Student
Advisor(s): Patrick Holland

https://twitter.com/ANagelski
@ANagelski

The active site clusters of nitrogenase enzymes have a C-based bridge between high-spin Fe sites. We present functional and structural models to elucidate the impacts of carbon and sulfide donors in simpler Fe compounds. This includes Fe alkyl and alkylidene complexes capable of reducing N_2 to NH_3 (with protons and electrons). We report the first diiron complex bridged by alkylidene and sulfide ligands, which models part of the active-site cluster (FeMoco) in the resting state of Mo-nitrogenase.

P110. Halogen Bonding as a Structure-Directing Interaction in Dithiadiazolyl Radicals

Mitchell Nascimento
University of Victoria, Victoria, Canada
Graduate Student
Advisor(s):

https://twitter.com/MitchellNas
@MitchellNas

We report dithiadiazolyl radicals p-XC_6F_4CNSSN (X = Br (1) or I (2)). 1 is polymorphic, comprising pure diamagnetic π^*-π^* dimers, fully monomeric radicals, and mixtures of each. 2 is isomorphous to 1α. Both Br and I groups in 1 and 2 promote sigma-hole interactions of the type C⋯N (X = Br, I), reflecting the strength of this interaction in heavier halo-derivatives. A subtle competition of halogen/nitrogen and sulfur/nitrogen bonds directs structure and is examined through DFT methods.

1. Nascimento, M. A.; Heyer, E.; Less, R. J.; Pask, C. M.; Arauzo, A.; Campo, J.; Rawson, J. M. *Cryst. Growth Des.* **2020**, 20, 4313.

P111. Olefin metathesis performance is impacted by X group reactivity in WOR_3X/SiO_2 catalysts

Chris Nicholas
Honeywell UOP, Des Plaines, United States
Industry
Advisor(s):

https://twitter.com/CatalysisChris
@CatalysisChris

The novel complex $W(=O)Np_3F$ has been synthesized and characterized by fluorination of the corresponding chloride counterpart with $AgBF_4$. Reaction with SiO_2 proceeds both through silanolysis and opening of a siloxane bridge thanks to the affinity of silicon for fluoride. This material presenting fluorine on its surface shows an enhanced catalytic activity in propylene self-metathesis in comparison to its monopodal counterpart $(SiO)W(=O)Np_3$.

1. Merle, N.; Mazoyer, E.; Szeto, K.C.; Rouge, P.; De Mallmann, A.; Berrier, E.; Delevoye, L.; Gauvin, R.M.; Nicholas, C.P.*; Basset, J.-M.*; Taoufik, M.* *J. Organomet. Chem.* **2018**, 869, 11-17.
2. Merle, N.; Girard, G.; Popoff, N.; De Mallmann, A.; Bouhoute, Y.; TreÌbosc, J.; Berrier, E.; Paul, J.-F.; Nicholas, C.P.; Del Rosal, I.; Maron, L.*; Gauvin, R.M.*; Delevoye, L.*; Taoufik, M.* *Inorg. Chem.* **2013**, 52, 10119-30.
3. Mazoyer, E.; Merle, Nicolas; de Mallmann, A.; Basset, J.-M.*; Berrier, E.; Delevoye, L.; Paul, J.-F.; Nicholas, C. P.; Gauvin, R. M.*; Taoufik, M.* *Chem. Commun.* **2010**, 46(47), 8944-8946.

P112. Imparting Multifunctionality by Utilizing Biporosity in a Zr-Based MOF

Pranay Ninawe
Indian Institute of Science Education and Research, Pune, India, Pune, India
Undergraduate Student
Advisor(s): Dr. Nirmalya Ballav

https://twitter.com/000pranay
@000pranay

An elegant design strategy of selectively incorporating conducting polymers in a bi-porous Metal-Organic Framework was introduced, which resulted in decoupled electrical and thermal conductivities. This process led to loading of ~12 wt% of polymers inside the pores. Electrical conductivity was enhanced by ~10^6 times in the nanocomposites bringing them into semiconducting regime, along with a significant decrease in thermal conductivity, as well as simultaneous porosity retention up to ~70%.

Jadhav, A.; Gupta, K.; Ninawe, P.; Ballav, N. *Angew. Chem. Int. Ed.* **2020**, 59, 2215.

P113. Activation of Ammonia and Hydrazine via the Formation of Terminal Fe(III) Amido and Imido Radical Intermediates

Lucie Nurdin
University of Calgary, Calgary, Canada
Graduate Student
Advisor(s): Prof. Warren Piers

https://twitter.com/lucie_nurdin
@lucie_nurdin

Herein, we explore the use of a dianionic pentadentate ligand B_2Pz_4Py reported by our group [1,2] for the activation of NH_3. We hypothesized that this robust and electronically rich ligand could help to stabilize higher oxidation state complexes. In particular, we sought to detect terminal Fe(III)NH_2 and Fe(IV)NH complexes as they have been proposed as key intermediates of ammonia oxidation to N_2, and could provide mechanistic insights to improve catalyst design using earth abundant metals.[3]

[1] Spasyuk, D. M.; Carpenter, S. H.; Kefalidis, C. E.; Piers, W. E.; Neidig, M. L.; Maron, L. *Chem. Sci.* **2016**, 7, 5939.
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[3] Zott, M. D.; Garrido-Barros, P.; Peters, J. C. *ACS Catal.* **2019**, 9, 10101.

P114. Biodegradable electronics: Ionic diode based on a cellulose nanocrystals-agarose hydrogel

Kudzanai Nyamayaro
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Prof Mehrkhodavandi

https://twitter.com/KudziNyamayaro
@KudziNyamayaro

Herein, we employ cellulose nanocrystals to fabricated a polyelectrolyte gel diode capable of rectifying ionic current. The current rectification ratio reaches 70 reproducibly, which is significantly higher than analogous diodes generated with microfibrillated cellulose (~15) and olefin based polyelectrolyte gel diode (~40). The current voltage characteristics of the CNC-hydrogel diode were influenced by concentration, gel thickness, scanning frequency, and applied voltage.

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2. Cayre, O. J.; Chang, S. T.; Velev, O. D., *J. Am. Chem. Soc.* **2007**, 129 (35), 10801-10806.

P115. Covalent Rigidification of Self-assembled Electroactive Materials with Polydiacetylenes

Audithya Nyayachavadi
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Simon Rondeau-Gagné

https://twitter.com/anyayach
@anyayach

Well-defined self-assembly of organic materials is an efficient strategy to control the optoelectronic properties of organic materials. However, supramolecular self-assembly are sometimes unstable and difficult to process. Here, we discuss our new approach to covalently stabilize self-assembled organic materials by incorporating diacetylenes capable of polymerizing in the solid state, preserving morphologies while tuning the optoelectronic properties of the resulting materials.

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2. Nyayachavadi, A.; Langlois, A.; Tahir, M. N.; Billet, B.; Rondeau-Gagné, S. *ACS Appl. Polym. Mater.* **2019**, 1, 1918.
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P116. Computatinal Design of Fluorescent Chemosensors for Mercury Detection: Binding Affinities of Metal Ions with Thiacrown Ether

Meagan Oakley
University of Minnesota, Minneapolis, United States
Post-doctoral Fellow
Advisor(s):

https://twitter.com/meaganoakley
@meaganoakley

Design and improvement of fluorescence-based chemosensors for the detection of heavy metals remains a challenge. We have studied the BODIPY-benzothiacrown chemosensor[1] which showed selective chelation-enhanced fluorescence to the Hg^{2+} metal ion. We computationally investigated the selectivity of the chemosensor as a positive fluorescent sensor for the Hg^{2+} metal, as well as considering other crown ethers and other metal ions in order to understand what drives the selectiveness of the crown.

[1] Kim, H.-J.; Kim, S.-H.; Kim, J.-H.; Lee, E.-H.; Kim, K.-W.; Kim, J. S. *Bull. Korean Chem. Soc.* **2008**, 29, 1831-1834.

P117. Pyrazine as Noncovalent Conformational Locks in Semiconducting Polymers for Enhanced Charge Transport and Stability in Thin Film Transistors

Michael Ocheje
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Simon Rondeau-Gagné

https://twitter.com/michocheje
michocheje

A backbone engineering was performed on highly rigid semiconducting polymers based on diketopyrropyrrole (DPP) units to include pyrazine-containing moieties. Their utilization in bottom-gate bottom-contact devices and their potential to act as ligands for coordinating metals highlights the capacity of this new semiconductor for fully printed high-performance electronics.

Ocheje, MU; Goodman, RB; St. Onge, PBJ; Malik, MN; Yadiki, M; He, Y; Tao, Y; Chu, TY; Rondeau-Gagné, S *J. Mat. Chem. C*, **2019**, 7, 11507

P118. Synthesis of bis(imidazolium) salts with dimethylene benzene linkers

Elisa Olivas
Cal State Polytechnic University, Bryn Mawr, United States
Undergraduate Student
Advisor(s): Dr. Chantal Stieber

https://twitter.com/ElisaOlivas4
@ElisaOlivas4

Bidentate N-heterocyclic carbene (NHC_2) ligands are of interest as strongly sigma-donating ligands to metals. Previous work illustrates NHC_2 ligands with primarily ethylene and methylene linkers. This work focuses on synthesis of conjugated (bis)imidazolium salts by reacting mesitylimidazole with 1,2-di(bromomethyl) benzene or 1,2-dibromo-2-phenylethane in toluene. Characterization was with X-ray diffraction and ^{1}H NMR. The NHC_2 with 1,2-di(bromomethyl) benzene was successfully synthesized.

Hopkinson, M. N.; Richter, C.; Schedler, M.; Glorius, F. An Overview of N-Heterocyclic Carbenes. *Nature* **2014**, 510 (7506), 485-496

P119. Luminescent Difluoroboron Complexes Supported by Phenanthridine-Based β-Ketoiminates

Robert Ortiz
University of Manitoba, Winnipeg, Canada
Undergraduate Student
Advisor(s): David Herbert

https://twitter.com/OrtizRobert44
@OrtizRobert44

Difluoroboron complexes have shown potential for developing cheaper materials for light emitting devices. Our group has developed synthetic methodologies that enable us to incorporate phenanthridine into various ligand frameworks, with their coordination complexes exhibiting interesting photophysical properties. Incorporating phenanthridine into β-ketoimines enabled us to isolate novel difluoroboron β-ketoiminates with photophysical properties dependent on the substituent on the phenanthridine.

P120. Controlled Generation of 9-Boratriptycene by Lewis Adduct Dissociation: Accessing a Non-Planar Triarylborane

Arnaud Osi
UNamur, Namur, Belgique
Graduate Student
Advisor(s): Prof. Guillaume Berionni

https://twitter.com/ArnaudOsi
@ArnaudOsi

The 9-boratriptycene was generated in solution by protodeboronation of a tetra-aryl boronate complex with HNTf$_2$. We studied its stereoelectronic properties by quantifying its association with Lewis bases. Beyond the high pyramidalization of the 9-boratriptycene and its low reorganization energy upon coordination, theoretical calculations revealed that the absence of π-donation from the triptycene aryl rings to the boron vacant p$_z$ orbital is the main reason for its high Lewis acidity.

Chardon, A.; Osi, A.; Mahaut, D.; Doan, T.-H.; Tumanov, N.; Wouters, J.; Fusaro, L.; Champagne, B.; Berionni, G. *Angew. Chem. Int. Ed.* **2020**, DOI: 10.1002/anie.202003119

P121. Boranes and Alanes: Novel Synthesis and Lactonisation

Darren Ould
Cardiff University, Wales
Graduate Student
Advisor(s): Rebecca L. Melen

https://twitter.com/darren_ould?lang=en
@darren_ould

Triaryl boranes have proven to be highly successful in catalysing organic reactions.[1,2] In this work the use of a series of triarylboranes to undergo metal-free lactonization of diazo compounds is presented, while also showing how tuning the Lewis acidity of the borane centre is important.[3] From here the synthesis and structural properties of a series of novel triarylalane species are discussed, highlighting key differences in the chemistry between triarylboranes and triarylalanes.[4]

[1] Lawson, J. R.; Melen, R. L. *Inorg. Chem.* **2017**, 56, 8627.
[2] Jupp, A. R. and Stephan, D. W., *Trends Chem.*, **2019**, 1, 35.
[3] Santi, M.; Ould, D. M. C.; Wenz, J.; Soltani, Y.; Melen, R. L.; Wirth, T. *Angew. Chem. Int. Ed.*, **2019**, 58, 7861.
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P122. Convenient Access to Germanium and Aluminium Compounds Using the Pendant Power of Methyl-pyridinato Ligand

SANJUKTA PAHAR
CSIR-NATIONAL CHEMICAL LABORATORY, Pune, India
Graduate Student
Advisor(s): Dr. Sakya Singha Sen

https://twitter.com/PaharSanjukta
@PaharSanjukta

A methyl-pyridine side arm in the nacnac, leads to a tridentate ligand (2,6-iPr$_2$-C$_6$H$_3$NC(Me)CHC(Me)NH(CH$_2$py)).We have synthesized and characterized chlorogermylene which undergoes unusual smooth ring contraction in presence of Lewis acid (GeCl$_2$) via C-N bond cleavage, facile dehydrocoupling and 6 membered Al-heterocycle. With another Lewis acid, AlCl$_3$, leads to the formation of dicholoaluminim complex via the transmetallation. Crystal reveals pyridine coordinates to the Al.

1. Xu, X.; Chen, Y.; Zou, G.; Sun, J. Single. *Dalton Trans.* **2010**, 39, 3952-3958
2. Pahar. S.; V.S.V.S.N. Swamy.; Das. T.; Gonnade. R. G.; Vanka. K.; Sen, S. S.; *Manuscript under preparation*

P123. Reactivity of Dioxygen and Nitric oxide towards Nonheme Diiron(II)-hydrosulfide Complex

Nabhendu Pal
Indian association for the cultivation of science, Kolkata, India
Graduate Student
Advisor(s): Dr. Amit majumdar

https://twitter.com/Nabhendupal
@nabhendupal

While attempted synthesis of diiron(II)-hydrosulfide complexes using HS-produced insoluble precipitate, Reaction of $Fe(BF_4)_2{\cdot}6H_2O$, Et_3N, and HN-Et-HPTB with RSH (R = $PhCH_2$,tBu) /NaStBu in DMF at RT yielded the desired complex. The dioxygen activity of 1a to generate an oxygenated diiron complex at low temperature and its subsequent decomposition at RT has been examined. The reaction of 1a with 6 eq. Ph_3CSNO produces $[Fe_2(N\text{-Et-HPTB})(SH)(NO)_2(DMF)](BF_4)^2$.

Pal. N; Majumdar. A; *Dalton Trans.* **2019**, 48, 5903-5908.

P124. High-throughput screening of MOF catalysts

Joseph Palomba
UC San Diego, San Diego, United States of America
Graduate Student
Advisor(s): Seth Cohen

https://twitter.com/PeriodiKangeroo
@PeriodiKangeroo

Metal-organic frameworks (MOFs) are microporous hybrid materials whose metal and organic components make them useful heterogeneous catalysts for chemical transformations. MOFs combine the recyclability of heterogeneous materials with active site tailoring akin to homogeneous catalysts. We developed a high-throughput screening (HTS) method to examine >100 MOFs and MOF-polymer composites. This HTS method was tested on chemical warfare agent simulants to probe a broad spectrum of chemical space.

P125. Rh(I) and Rh(III) pincer complexes: (R,R)-Ph-pybox vs iPr-PNP

Gemma Parker
University of Warwick, Coventry, United Kingdom
Graduate Student
Advisor(s): Adrian Chaplin

https://twitter.com/GemmaParker0110
@GemmaParker0110

Pincer ligands are frequently used in organometallic chemistry and can be readily adapted, enabling the steric and electronic properties of metal derivatives to be tuned.(1) However, the impact of such changes can be difficult to gauge in a quantitative manner. To this end, we present our work investigating the rhodium(I) and rhodium(III) carbonyl fragments as probes for the donor properties of pincer ligands, exploiting convenient spectroscopic handles.(2)

1. E. Peris and R. H. Crabtree, *Chem. Soc. Rev.*, **2018**, 47, 1959-1968.
2. G. L. Parker, S. Lau, B. Leforestier and A. B. Chaplin, *Eur. J. Inorg. Chem.*, **2019**, 3791-3798.

P126. Heavy main-group carbonyl-alkyne metathesis

Löwe Pawel
Westfälische Wilhelms-Universität Münster, Münster, Germany
Graduate Student
Advisor(s): Dr. Fabian Dielmann

https://twitter.com/PawelLoewe
@PawelLoewe

On this poster we show that oxophosphonium ions, which are the isoelectronic phosphorus congeners to carbonyl compounds, undergo [2+2] cycloaddition reactions with different terminal alkynes to generate cationic 1,2-oxaphosphetes. This new compound class was isolated and structurally characterized. The strained phosphorus-oxygen heterocycles open to the corresponding hetero-diene structure at elevated temperature, which was used to generate six-membered phosphorus heterocycles.

P. Löwe, M. Feldt, M. A. Wünsche, L. F. B. Wilm, F. Dielmann *J. Am. Chem. Soc.* **2020**, 142, 21, 9818-9826.

P127. How Does Milstein’s Catalyst Really Work?

John Pham
Colgate University, Hamilton, NY, United States
Undergraduate Student
Advisor(s): Anthony Chianese

https://twitter.com/jjrpham
@jjrpham

Mechanistic proposals of Milstein’s ruthenium pincer catalyst for ester hydrogenation have relied on reversible deprotonation of a methylene linker of the pincer ligand. Here, we present evidence that under catalytic conditions, Milstein’s catalyst undergoes ethane loss followed by hydrogen addition to give an active catalyst containing an N-H group. This newly discovered activated form is the most efficient catalyst for ester hydrogenation, giving over 10,000 turnovers at rt with no added base.

P128. Conversion of amine from aromatic nitro compounds using Heterogeneous catalyst

Ariprasanth Ramalingam
SRM University, Chennai, India
Graduate Student
Advisor(s): Prof.M.Sasidharan

https://mobile.twitter.com/ARIPRASANTH4
Ariprasanth 4

The reduction of aromatic nitro compound to amines is an important organic transformation. As amines are necessary for preparation of dye, drugs, herbicides, and pesticides and preparation of amines received great attention Here we demonstrate the synthesis of amines from nitro compounds using base metal catalysts. The catalysts were thoroughly investigated by a series of characterization techniques such as XRD, TEM, SEM, and XPS.

P129. Stabilization and significance of group 14 metallylenes

Ravindra Raut
Indian Institute of Science Education and Research, Pune, Pune, India
Graduate Student
Advisor(s): Dr. Moumita Majumdar

https://twitter.com/ravindraraut19
@ravindraraut19

The heavier analogues of carbene are unique due to its one unoccupied and another lone pair orbital, which can mimic the transition metals. The stabilization of such challenging species either requires steric protection by bulky ligand or kinetic stabilization by extra donor group in ligand. Here, we have stabilized neutral and cationic forms of germylenes and stannylene in simple Schiff base multidentate ligands. The unusual reactivity is displayed in the current poster.

P130. Cationic Alkyl-Indium Complexes: Tuning the Reactivity with Hemilability

Hootan Roshandel
University of British Columbia, Vancouver, Canada
Undergraduate Student
Advisor(s): Prof. Parisa Mehrkhodavandi

https://twitter.com/hootan_r
@hootan_r

Although widely used to tune the chemistry of transition metals, there are only a handful of reported hemilabile systems that explore the reactivity of group-13 metals. Thus, based on previous work in our group, we developed a series of cationic alkyl-indium complexes containing a heterocyclic hemilabile side-arm, providing the first glance at using hemilability to significantly influence the reactivity of indium complexes towards the ring opening polymerization of epoxides and rac-lactide.

1. Jung, H.-J.; Chang, C.; Yu, I.; Aluthge, D. C.; Ebrahimi, T.; Mehrkhodavandi, P., *ChemCatChem* **2018**, 10 (15), 3219-3222.
2. Diaz, C.; Ebrahimi, T.; Mehrkhodavandi, P.. *Chem. Commun.* **2019**, 55 (23), 3347-3350.

P131. Computational Insight into the Sulfilimine (S=N) Bond Formation in Collagen-IV.

Anupom Roy
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): James W. Gauld

https://twitter.com/Anupom88
@Anupom88

Collagen IV is an essential component of the basement membrane in the tissues. It provides proper cellular structure by the formation of sulfilimine bond (S=N) between Methionine and Lysine or Hydroxylysine (cross-links) residues which can be formed with or without post-translational modification. The aim of the study is the investigation of the formation of sulfilimine bond and its nature in Collagen IV using multi-scale approach that included MD, QM-Cluster, QT-AIM, and NBO analysis.

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2. Vanacore, R., Ham, A.J.L., Voehler, M., Sanders, C.R., Conrads, T.P., Veenstra, T.D., Sharpless, K.B., Dawson, P.E. and Hudson, B.G. *Science* **2009** 325, 1230-1234.

P132. Electrically Conductive and Photosensitive Heteronuclear Complexes: From Binuclear to Tetranuclear to Coordination Polymers.

Sourav Roy
Indian Institute of Science, India
Post-doctoral Fellow
Advisor(s):

https://twitter.com/souravscott
@souravscott

Recently inorganic-organic hybrids are found to be useful for the fabrication of active electronic devices.[1-4] Two Ni/Pb, one Co/Na and one Co/Hg/Na Schiff base complexes are prepared and their electrical properties are investigated which show significant on-off ratio when used as photo-switch. Unique supramolecular networks [C-H···π(N3) and S···Br interactions] are observed in the complexes which can modulate the electrical conductivities.[5]

1) Dey, A.; Layek, A.; Roychowdhury, A.; Das, M.; Datta, J.; Middya, S.; Das, D.; Ray, P. P. *RSC Adv.* **2015**, 5, 36560.
2) Roy, S.; Halder, S.; Drew, M. G. B.; Ray, P. P.; Chattopadhyay, S. *New J. Chem.* **2018**, 42, 15295.
3) Roy, S.; Halder, S.; Drew, M. G. B.; Ray, P. P.; Chattopadhyay, S. *ACS Omega* **2018**, 3, 12788.
4) Roy, S.; Dey, A.; Ray, P. P.; Ortega-Castro, J.; Frontera, A.; Chattopadhyay, S. *Chem. Commun.* **2015**, 51, 12974.
5) Conesa-Egea, J.; Redondo, C. D.; Martinez, J. I.; Gomez-Garcia, C. J.; Castillo, O; Zamora, F.; Amo-Ochoa, P. *Inorg. Chem.* **2018**, 57, 7568.

P133. Photocatalytic hydrogen evolution under red light using ruthenium(II) 2,4-di(pyridin-2-yl)-pyrimidine complexes as photosensitizers

Mira Rupp
Université de Montréal, Universitaet Wuerzburg, Montréal, Canada
Graduate Student
Advisor(s): Garry Hanan; Dirk Kurth

https://twitter.com/MiraRupp
@MiraRupp

A series of non-symmetric 2,6-di(pyridin-2-yl)-pyrimidine ligands with peripheral pyridine substituents in different positions and their Ru(II) complexes are reported. They exhibit a red-shifted emission, longer excited-state lifetimes and higher luminescence quantum yields and are easier to reduce than analogous terpyridine (tpy) complexes. In H_2 evolution experiments under blue and red light, the complexes are more active but less stable than previously reported $[Ru(tpy)2]^{2+}$ photosensitizers.

P134. Synthesis and Reactivity of a Terminal Gallium Imide

Artemis Saddington
University of Oxford, Oxford, United Kingdom
Undergraduate Student
Advisor(s): Simon Aldridge

https://twitter.com/artemis_sadd
@artemis_sadd

The potassium gallyl complex $K_2[(NON)Ga]_2$ (NON = 4,5-bis(2,6-diisopropylanilido)-2,7-ditertbutyl-9,9-dimethylxanthene) acts as a source of nucleophilic gallium. The reaction of $K_2[(NON)Ga]_2$ with the bulky azide Ph_3SiN_3 enables the isolation of a terminal gallium imide species. The imide contains a highly polarised Ga-N bond, enabling reaction with PhCCH, $PhSiH_3$, PhCHO, CO_2, N_2O and CO.

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2. Heilmann, A.; Hicks, J.; Vasko, P.; Goicoechea, J.; Aldridge, S. *Angew. Chemie. Int. Ed.* **2020**, 132, 4927-4931.

P135. Commodity Polymers to Functional Materials: Single Step Synthesis via Hydroaminoalkylation

Sabrina Scott
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Laurel Schafer

https://twitter.com/sabselscott
@sabselscott

In an effort to improve the accessibility of functional materials, vinyl terminated polypropylene was aminated via the atom-economic hydroaminoalkylation transformation in solvent free conditions. This work provides an inexpensive and resource conscious protocol to access mono-telechelic polymers with amine functionality, providing an alternative to the typical multi-step syntheses often coupled with protection/deprotection procedures which fail to meet modern demands for “green” products.[1-5]

1. J. Y. Dong, Z. M. Wang, H. Hong and T. C. Chung, *Macromolecules*, **2002**, 35, 9352-9359.
2. S. Ji, T. R. Hoye and C. W. Macosko, *Polymer*, **2008**, 49, 5307-5313.
3. A. A. Nagarkar, A. Crochet, K. M. Fromm and A. F. M. Kilbinger, *Macromolecules*, **2012**, 45, 4447-4453.
4. S. Pal, F. Lucarini, A. Ruggi and A. F. M. Kilbinger, *J. Am. Chem. Soc*, **2018**, 140, 3181-3185.
5. M. Alizadeh and A. F. M. Kilbinger, *Macromolecules*, **2018**, 51, 4363-4369.

P136. Electronic structure investigation of electron rich and deficient Cu-salen complexes

Anmol Sharma
University of the Fraser Valley, Abbotsford, Canada
Undergraduate Student
Advisor(s): Linus Chiang

https://twitter.com/anmol98z
@anmol98z

Metal complexes coordinated by salen ligands have attracted much attention due to their highly tunable nature and consequently diverse application in catalysis and medicinal purposes.[1-3] This poster will discuss the synthesis of three novel Cu-salen complexes and characterization via IR, UV-Vis, and NMR spectroscopies. The electronic structure of the target compounds, investigated by cyclic voltammetry, will also be discussed.

1 - Chiang, L., Herasymchuk, K., Thomas, F., Storr, T., *Inorg. Chem.*, **2015**, 54, 5970-5980
2 - Kanso, H., Clarke, R. M., Kochem, A., Arora, H., Philouze, C., Jarjayes, O., Storr, T., Thomas, F., *Inorg. Chem.*, **2020**, 59, 5133-5148
3 - Bellefeuille, D., Orio, M., Barra, A., Aukauloo, A., Journaux, Y., Philouze, C., Ottenwaelder, X., Thomas, F., *Inorg. Chem.*, **2015**, 54, 9013-9026

P137. Oligonuclear Ru(II) Assemblies Based on Ditopic Terpyridine Ligands

Natali Shevchenko
Université de Montréal, Montréal, Canada
Undergraduate Student
Advisor(s): Garry S. Hanan

https://twitter.com/NataliShevche15
@NataliShevche15

Linear polytopic terpyridine ligands can form rod-type assemblies when complexed with metal ions like ruthenium and iron. In this study, ditopic terpyridine ligands are synthesized, complexed and characterized. Tertbutyl groups are introduced to the ligands to increase the solubility of long supramolecular assemblies in organic solvents. The complex’s absorption and redox potentials are studied and compared to an iron complex of the monotopic terpyridine ligand with tertbutyl substituents.

1. T. Auvray, R. Sahoo, D. Deschenes, G. S. Hanan, *Dalton Trans.*, **2019**, 48, 15136-15143
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3. D. J. Diaz, S. Bernhard, G. D. Storrier, H. D. Abruna, *J. Phys. Chem. B*, **2001**, 105, 8746-8754.
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P138. Terphenyl(bisamino)phosphines as Ligands in Gold-Catalysis

Jan-Erik Siewert
LIKAT Rostock, Rostock, Germany
Undergraduate Student
Advisor(s): Christian Hering-Junghans

https://twitter.com/siewert_jan
@siewert_jan

Terphenyl(bisamino)phosphines have been identified as effective ligands in cationic gold(I) complexes for the hydroamination of acetylenes. These systems are related to Buchwald phosphines and their steric properties have been evaluated. Effective hydroamination was noted even at low catalyst loadings and a series of cationic gold(I) complexes has been structurally characterized clearly indicating stabilizing effects through gold-arene interactions.

1. D. S. Surry, S. L. Buchwald, *Angew. Chem., Int. Ed.* **2008**, 47, 6331.
2. D. Malhotra, M. S. Mashuta, G. B. Hammond, B. Xu, *Angew. Chem., Int. Ed.* **2014**, 53, 4456.
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P139. Cytotoxic activity studies against non-tumorigenic HEK293 and cancer HEPG2 cell lines by Vanadium (V) compounds

Aniela Silva Nolasco
Universidad Juarez Autonoma de Tabasco, Tabasco, México
Graduate Student
Advisor(s): Irma Sanchez Lombardo

https://twitter.com/anni_nolasco
anni_nolasco

Recent studies have established the ability of decavanadates that contain amine-based ligands and/or cations to exert different biological effects in vitro and in vivo.[1-3] In this study the cytotoxic activity studies against non-tumorigenic HEK293 human embryonic kidney cells and human liver cancer HEPG2 cells (IC 50 values) were performed for sodium decavanadate, metforminium decavanadate, sodium metavanadate and metformin hydrochloride in a concentration range of 10-100 μM.

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4. Sanchez, I. et al. *Eur J. Inorg. Chem.* **2014**, 27, 4581.

P140. Analysis of Solid-State Geometries and Ground-State Energies of Tin-Containing Complexes via DFT

Kaitlyn Silverthorne
Ryerson University, Toronto, Canada
Undergraduate Student
Advisor(s): Dr. Daniel Foucher

https://twitter.com/silverthornekt
@silverthornekt

Polystannanes are of interest due to their low band-gap and semi-conductive properties. Several monomeric precursors have been synthesized and characterized via NMR (^{119}Sn) spectroscopy and single-crystal XRD. My project focuses on analyzing these tin-containing small molecules via DFT to assess the accuracy of various functionals in predicting solid-state geometries and ground-state energies of both the open and hypercoordinate conformations of these complexes.

1. Pau, J.; D'Amaral, G. M.; Lough, A. J.; Wylie, R. S.; Foucher, D. A. *Chem. Eur. J.* **2018**, 24, 18762-18771

P141. Iron catalyzed hydroboration of alkenes and alkynes

Arpita Singh
Texas Tech University, Lubbock, United States
Graduate Student
Advisor(s): Dr. Michael Findlater

https://twitter.com/Arpita1391
@Arpita1391

Iron complexes [BIAN]Fe(I)(toluene) and [BIAN]$FeCl_2$ (BIAN=bis(2,6-diisopropylaniline)acenaphthene) have been employed in the selective reduction of alkynes and alkenes via hydroboration. The hydroboration of alkynes and alkenes in the presence of HBpin and an activator at 70 °C afforded linear vinyl and alkyl boronic esters, respectively. Selectivity up to 98% was observed for alkyl boronic esters and exclusive formation of trans product was observed for vinyl boronic esters.

P142. Small Molecule Activation by Transition Metal Polyhydride Clusters

Kathleen Snook
Boston University, Boston, United States
Undergraduate Student
Advisor(s): John Caradonna

https://twitter.com/asexualchemist1
asexualchemist1

Polyhydride transition metal clusters introduce a new type of catalyst with multiple reactive metal surfaces, reservoirs of electron density, and fluxional hydride ligands. We are investigating the topology of an open butterfly cluster $[M_4(\mu_3\text{-}X)_2(\mu\text{-}X)_5X_4]^{n-}$ along with the hexatungsten clusters $[W_6(\mu_3\text{-}Cl)_8Cl_6]^{2-}$ and $[W_6(\mu\text{-}Cl)_{12}Cl_6]^{2-}$. Successful syntheses of these clusters are confirmed by Raman and ^{183}W NMR spectroscopy, and SCXD studies.

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3. *Energy Fuels*. **2009**, 23 (4), 1874-1887.
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5. *J. Am. Chem. Soc.* **1982**, 104 (21), 5630-5633.
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P143. A Responsive-at-Metal Cyclometalated Platinum Luminophore

Miguel Soto
University of British Columbia, Vancouver, Canada
Post-doctoral Fellow
Advisor(s): Mark MacLachlan

https://twitter.com/Miguel_A_Soto_
@Miguel_A_Soto_

Molecular emitters are very valued as they are used in a range of applications and technologies. When designing an emitter, there are three characteristics that are highly desirable to control: emitted color, emission decay, and quantum yield, which are adjusted through the selection of a metal core, and by the covalent modification of a ligand. Here, I will discuss how simple solvent molecules can get the job done by modulating non-covalent interactions in cyclometalated Pt(II) complexes

Soto, M. A.; Carta, V.; Andrews, R. J.; Chaudhry, M. T.; MacLachlan, M. J., *Angew. Chem. Int. Ed.* **2020**, 59, 10348

P144. Tuning the Redox Properties of MnI-NHC Complex Through Remote Coordination Approach

Anandi Srinivasan
Laboratoire d'Electrochimie Moléculaire LEM, Paris, Paris, France
Post-doctoral Fellow
Advisor(s): Dr. Orestes Rivada Wheelghan

https://twitter.com/AnandiSrinivas1
@AnandiSrinivas1

Modulating the electronics and reactivity of transition metal complexes by incorporating alkali metal substituents offers a powerful strategy for enhancing the performance electrocatalysts. Along these lines, we present the correlation of remote interactions of different alkali cations with the novel MnI complex, 1, and its effects on the redox behavior of Mn center. Additionally, the electrochemical behavior of 1 towards CO_2, including the effects of added alkali salts will be presented

P145. Optimizing Semiconducting Materials Through M-L Interactions.

Blake St. Onge
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Simon Rondeau-Gagne

https://twitter.com/stonge912
@Stonge912

Metal-Ligand (M-L) interactions in materials chemistry which involve the incorporation of side-chain engineering in semiconducting π-conjugated polymers have become an increasingly popular field of study. Our work concludes that utilizing semiconducting π-conjugated polymers with pincer ligands in the sidechains can incorporate Fe(II) centers which demonstrate an increase in device performance and mobilities.

P. B. St.Onge, T. Chen, A. Langlois, A. Younus, I. Jo Hai, B. Lin, Y. Chiu and S. Rondeau-Gagné, *J. Mater. Chem. C.* **2020**, DOI: 10.1039/D0TC01536A.

P146. Synthesis of Redox Active Organoindium Dithiolate Catalysts

Alexander Stöckli
Mount Allison University, Sackville, NB, Canada
Undergraduate Student
Advisor(s): Glen Briand

https://twitter.com/HubertStockli
@HubertStockli

Traditional redox catalysts use precious transition metals and tend to produce toxic waste. Use of relatively non-toxic indium as a metal centre in these compounds would help alleviate this problem. However, indium has limited redox activity on its and so the use of a redox active ligand is needed. This work seeks to synthesize redox active indium compounds with varied physical properties. The synthesis and structural characterization of a novel indium 3,4-toluenedithiolate complex is reported.

P147. C-C Bond Formation Reactions Using $B(C_6F_5)_3$

Katarina Stefkova
Cardiff University, Cardiff, United Kingdom
Graduate Student
Advisor(s): Dr. Rebecca Melen

https://twitter.com/KatarinaStefko1
@KatarinaStefko1

The poster demonstrates the recent developments in $B(C_6F_5)_3$ catalysed alkenylations as well as it shows the utilization of $B(C_6F_5)_3$ with $PMes_3$ as Frustrated Lewis Pairs in higly stereoselective C-C bond formation to obtain E- alkenes from readily available styrenes.

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P148. C(sp^2)-C(sp^2) homo-dimerization of a pincer scaffold: A synergistic experimental and computational study supports binuclear Ni(III)-Ni(III) mechanisms

S. Maryamdokht Taimoory Taimoory
University of Michigan, Chemistry Department, Ann Arbor, USA
Post-doctoral Fellow
Advisor(s): Prof. Melanie S. Sanford

https://twitter.com/NTaimoory
@NTaimoory

Chemical transformations promoted by bimetallic systems are abundant in nature and catalytic processes.[1,2] This presentation will highlight our ongoing studies on of the key role of bimetallic Ni(III)-Ni(III) complexes in mediating the C(sp^2)-C(sp^2) reductive elimination on a catalytically relevant, quinoline-benzamide scaffold.

1. Lindahl, et. al. *J. Inorg. Biochem*. **2012**, 106, 172.
2. a) Diao et. al. *J. Am. Chem. Soc.* **2016**, 138, 4779; b) Diao et. al. *Angew. Chem. Int. Ed.* **2016**, 55,7534; c) Uyeda et. al. *ACS Catal.* **2017**, 7, 936; d) Ritter et. al. *J. Am. Chem. Soc.* **2012**, 134, 12002.

P149. Ni-salen complexes bearing pendant phenol groups in the secondary coordination sphere

Kaeden Teindl
University of the Fraser Valley, Abbotsford, Canada
Undergraduate Student
Advisor(s): Linus Chiang

https://twitter.com/KTeindl
@KTeindl

The secondary coordination sphere (SCS) often plays an essential role in enzymatic processes,[1] which has inspired efforts to integrate SCS design into synthetic targets.[2-4] To that end, this poster will discuss the synthesis and spectroscopic characterization of novel nickel-salen complexes with phenol moieties appended in their SCS.[5] Their electrochemical behaviors were probed by CV, and the subsequent one-electron oxidized species were prepared and investigated spectroscopically.

1. Jeoung, J.-H.; Dobbek, H. *Science* **2007**, 318, 1461-1464
2. Sun, P; Yang, D; Li, Y; Wang, B; Qu, J. *Dalton Trans.* **2020**, Advance Article
3. Hong, D; Kawanishi, T; Tsukakoshi, Y.; Kotani, H.; Ishizuka, T.; Kojima, T. *J. Am. Chem. Soc.* **2019**, 141, 20309-20317
4. Wijeratne, G.B.; Bhadra, M.; Siegler, M.A.; Karlin, K.D. *J. Am. Chem. Soc.* **2019**, 141, 17962-17967
5. Chiang et al. *Chem. Eur. J.* **2012**, 18, 14117 - 14127

P150. Structural Landscape of Lanthanide coordinated Anderson-Evans polyoxometalate

Shailabh Tewari
Indian Institute of Technology, Delhi, New Delhi, India
Graduate Student
Advisor(s): Arunachalam Ramanan

https://twitter.com/ShailabhTewari
@ShailabhTewari

The struggle in rationalizing crystallization, a supramolecular reaction, for the targeted design of functional materials is to recognize the underlined possible pathways. The task is significantly challenging due to the obscurity of well-defined links between synthesis, structure and property. However, Polyoxometalates (POM), the intermediate soluble molecular analogues of the bulk oxides, may provide some insights.

1. Tewari, S. et al. *Front. Chem.* **2019**, 6, 635.

P151. Gas phase characterization of a dinitrogen analogue of Zeise's salt

Gilian Thomas
University of Victoria, Victoria, Canada
Graduate Student
Advisor(s): Prof. Scott McIndoe

https://twitter.com/gilian_thomas
@gilian_thomas

We discovered a derivative of Zeise's salt ($[PtCl_3(C_2H_4)]^-$), the $[PtCl_3(N_2)]^-$ complex spontaneously forms in the nitrogen-rich atmosphere of the mass spectrometer. Ion mobility separation of $[PtCl_3(C_2H_4)]^-$, $[PtCl_3(N_2)]^-$ and $[PtCl_3(CO)]^-$, and MS/MS experiments analyzed ligand binding strength for the isobaric complexes. These were in agreement with calculated values. Binding strength may allow $[PtCl_3(N_2)]^-$ to be isolated with the potential for dinitrogen functionalization and catalysis in water.

P152. Impact of Sterics and Metal Choice on Isostructural Group VI Alkyne Metathesis Catalysts and the Selective Formation of Isomeric Metallacyclic Intermediates.

Richard Thompson
Louisiana State University, Baton Rouge, United States
Post-doctoral Fellow
Advisor(s): Semin Lee

https://twitter.com/RichardRThomps1
@RichardRThomps1

Metallacyclobutadienes as part of a cycloaddition based mechanism for alkyne metathesis is an established paradigm with alternate species viewed as decomposition products. Recently we reported the exclusive formation of a dynamic metallatetrahedrane capable of metathesis raising question about the mechanism. Consequentially, we report the synthesis a library of both molybdenum and tungsten alkylidynes supported by sterically distinct ligands and the role metal identity has on intermediates.

Thompson, R. R.; Rotella, M. E.; Du, P.; Zhou, X.; Fronczek, F. R.; Kumar, R.; Gutierrez, O.; Lee, S., *Organometallics* **2019**, 38, 4054-4059.

P153. Trans oxidative addition of arylfluorides to nickel N-heterocyclic carbene complexes

Adrian Torres
Cal State Polytechnic University, Pomona, Pomona, United States
Undergraduate Student
Advisor(s): Dr. S. Chantal E. Stieber

https://twitter.com/AdrianChem
@AdrianChem

Nickel N-heterocyclic carbene (NHC) complexes with isopropyl groups were reported to yield trans addition of aryl fluorides. In this work, NHC ligands with methyl groups were studied for oxidative addition of aryl fluorides at nickel. The aryl fluoride nickel complex was obtained from an oxidative addition of hexafluorobenzene to the nickel(0) precursor. Complexes were characterized using NMR spectroscopy and X-ray crystallography. A trans addition product was observed for the methyl complex.

1) Schaub, T.; Backes, M.; Radius, U. Square-Planar (Pentafluorophenyl)Nickel(II) Complexes by Derivatization of a C-F Activation Product. *Eur. J. Inorg. Chem.* **2008**, 2008 (17), 2680-2690. https://doi.org/10.1002/ejic.200800213.

P154. Clays modified with [Fe(o-phen)$_3$]$^{2+}$ complex for the removal of triclosan from aqueous solutions

Carlos Torres-Méndez
Escuela de Quimica, Facultad de Ciencias Quimicas y Farmacia, Universidad de San Carlos de Guatemala, Guatemala, Guatemala
Undergraduate Student
Advisor(s): PhD. Silvia EcheverrÃ¬a

https://twitter.com/randomrandom901
@randomrandom901

Bentonite (Bent) and vermiculite (Vrm) were modified by ionic exchange with [Fe(o-phen)$_3$]SO_4 complex. The modified clays showed a change of color to an intense red, characteristic of [Fe(o-phen)$_3$]$^{2+}$ complex. Materials were characterized by ATR FTIR, the hybrid clays showed bands at 720, 848, 1428 cm^{-1} assigned to bending vibrations of C-H bonds in the aromatic rings of the o-phen ligand. Comparative analysis on isotherms and the sorption capacity of Bent, Verm and hybrid clays is presented.

(1) Lei, C.; Hu, Y.; He, M. *Chem. Eng. J.* **2013**, 219, 361-370.
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(4) Chen, X. *Information* **2015**, 6 (1), 14-22.

P155. Application of FLP Chemistry to Reactions with Bromoalkynes

Jonah Toth
University of Toronto, Toronto, Canada
Undergraduate Student
Advisor(s): Douglas W. Stephan

http://twitter.com/jonahtoth
@jonahtoth

It was previously reported that sterically encumbered or electron deficient phosphines do not react with (bromoethynyl)benzene.[1] Our work has involved a systematic study of the reactivity induced by Lewis acids of varied strength to promote reaction between haloalkynes of the form RCCBr and a range of phosphines bearing either bulky or electron-withdrawing substituents. This study represents the first known application of FLP chemistry involving bromoalkyne substrates.

[1] Veinot, A.J.; Todd, A.D.K.; Robertson, K.N.; Masuda, J.D. *Can. J. Chem.* **2017**, 96, 8-17.

P156. Development of Cu-pyridinedicarboxamide Complexes as C-H Bond Activation Reagents

Warren VandeVen
University of the Fraser Valley, Abbotsford, Canada
Undergraduate Student
Advisor(s): Linus Chiang

https://twitter.com/VandevenWarren
@VandevenWarren

Nature utilizes high valent metal centers in enzymes to functionalize relatively inert C-H bonds.[1-2] Synthetic Cu(III) complexes, ligated by a dianionic, tridentate pyridinedicarboxamide (PCA) ligand, have demonstrated success in such reactions.[3-4] This poster will discuss the synthesis and characterization of a Cu complex ligated by an electron-rich PCA ligand. A more electron donating ligand is expected to stabilize the Cu(III) metal center, improving C-H bond activation reactivity.

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P157. The path from darkness to light: octahedral iridium(III) complexes to combat cancer.

Gloria Vigueras
University of Murcia, Murcia, Spain
Graduate Student
Advisor(s): José Ruiz López (@jruizum)

https://twitter.com/ViguerasGloria
@ViguerasGloria

We will present our recent results on the synthesis and biological evaluation of different bis-cyclometalated Ir(III) complexes.[1-3] Modifying the cyclometalated ligand and/or ancillary ligand we can tuned their antitumoral activity. Thus, some of them are very active in several cancer cell lines in the dark while others, are able to activate by irradiation with visible light.

1. Yellol, J.; Pérez, S. A.; Yellol, G.; Zajac, J.; Donaire, A.; Vigueras, G.; Novohradsky, V.; Janiak, C.; Brabec, V.; Ruiz, J. *Chem. Commun.* **2016**, 52, 14165.
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P158. Investigations into the polymerization mechanism and reactivity of 1-phosphabutadienes

Henry Walsgrove
University of British Columbia, Vancouver, Canada
Graduate Student
Advisor(s): Derek Gates

https://mobile.twitter.com/HWalsgrove
@HWalsgrove

We recently reported the polymerization of 1-phosphaisoprene by anionic initiation.[1] Studies of the polymer microstructure showed predominantly 3,4-addition across the C=C double bond, forming a polymer containing pendant phosphaalkene groups. Initiation studies using ^{n}BuLi show a 4,1-enchainment, in contrast to the proposed polymer microstructure resulting from 4,3-addition. Further investigation of the reactivity of 1-phosphabutadiene species will also be presented.[2,3]

1. Dück, K.; Rawe, B. W.; Scott, M. R.; Gates, D. P. *Angew. Chem. Int. Ed.* **2017**, 56, 9507.
2. Ohtsuki, K.; Walsgrove, H. T. G.; Hayahsi, Y.; Kawauchi, S.; Patrick, B. O.; Gates, D. P.; Ito, S. *Chem. Commun.* **2020**, 56, 774.
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P159. Supramolecular Capsules from Iso-Chalcogenazole N-Oxides

JinZhao Wang
McMaster University, Hamilton, Canada
Graduate Student
Advisor(s): Dr.Ignacio Vargas-Baca

https://twitter.com/zoomjin19
@zoomjin19

Amongst the many molecules that are capable of forming chalcogen bonds, iso-tellurazole N-oxides stand out because of their ability to reversibly form macrocyclic aggregates that are persistent in solution[1,2]. In recent investigations, we have found a procedure that builds a dodecamer that folds onto itself forming a cavitand that encapsulates certain molecules such as cyclohexane, tetrahydrofuran and dioxane.

1. P.C. Ho, P. Szydlowski, J. Sinclair, P. J. W. Elder, J. Kübel, C. Gendy, L. Myongwon Lee, H. Jenkins, J. F. Britten, D. R. Morim, I. Vargas-Baca. *Nature* Commun. **2016**, 7:11299.
2. P.C. Ho, J. Rafique, L. M. Lee, H. A. Jenkins, J. F. Britten, A. L. Braga, I. Vargas-Baca.* *Dalton Trans.*, **2017**, 46, 6570-6579.

P160. Oxidative addition reactions of tetrathiocins to group 10 metals: From structural diversity to sensor development.

Lara Watanabe
University of Windsor, Windsor, Canada
Graduate Student
Advisor(s): Dr. Jeremy Rawson & Dr. Charles Macdonald

https://twitter.com/larawatanabe
@larawatanabe

Metal dithiolene complexes are ideal for various materials applications. Oxidative addition reactions of bis(benzo)-1,2,5,6-tetrathiocins to zero valent group 10 metal complexes leads to mono-, di- and hexa-nuclear complexes depending on the steric effects of the phosphine. We have exploited this synthetic methodology to provide a simple two-step route to functionalized dithiolate complexes that we can explore as sensors for Na^+ cations.

1. Dithiolene chemistry: *Synthesis*, properties, and applications, ed. E. I. Stiefel, Interscience, Hoboken, New Jersey, **2003**.
2. Wrixon, J.; Hayward, J.; Raza, O.; and Rawson, J. M., *Dalton Trans.* **2014**, 43, 2134.
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4. Watanabe, L. K.; Wrixon, J. D.; Ahmed, Z. S.; Hayward, J. J.; Abbasi, P.; Pilkington, M.; Macdonald, C. L. B., and Rawson, J. M., *Dalton Trans.*, **2020**, DOI: 10.1039/D0DT01678K.

P161. Synthesis, characterization and cytotoxicity studies of multinuclear benzimidazole-based cyclometallated and cationic ruthenium(II) complexes

Athi Welsh
University of Cape Town, Cape Town, South Africa
Graduate Student
Advisor(s): Assoc. Prof. Gregory S. Smith

https://twitter.com/athiwelsh
@athiwelsh

In this study, a series of trimeric benzimidazole ligands, and their respective trinuclear Ru(II) complexes were synthesized and screened for their anticancer activity against two breast cancer cell lines. Overall, the compounds show anticancer activity either comparable to or greater than that of cisplatin. Importantly, the compounds have relatively low toxicity towards the non-tumorigenic cells and were noted to be significantly more selective for breast cancer cells compared to cisplatin.

A. Welsh, L. Rylands, V. B. Arion, S. Prince and G. S. Smith, *Dalton Trans.*, **2020**, 49, 1143 - 1156.

P162. Examination of the Effects of Solvents on Homogeneous CO_2 Reduction Electrocatalysis

Lucienna Wolf
DePaul University, Chicago, United States
Undergraduate Student
Advisor(s): Kyle A. Grice

https://twitter.com/LucyWol58238133
@LucyWol58238133

Significant effort has been focused on designing more efficient catalysts for CO_2 reduction, yet there is minimal information regarding the effects of solvent environments on these systems. Electrochemical and spectroscopic data collected from experiments using the canonical fac-Re(bpy)(CO)$_3$Cl electrocatalyst in various solvents were compared to the solvents' physical properties and their economic and environmental properties to determine the most optimal conditions for CO_2 reduction systems.

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2. Lu, Q.; Jiao, F., Electrochemical CO_2 reduction: Electrocatalyst, reaction mechanism, and process engineering. **2016**; Vol. 29.
3. Grice, K. A.; Saucedo, C., *Inorganic Chemistry* **2016**, 55, 6240-6246.
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5. Gutmann, V. (1978) The donor-acceptor aproach to molecular interactions. New York: Plenum Press. 6. Dean, J. A.; Lange, N. A., Lange's handbook of chemistry. 15th ed. ed.; McGraw-Hill: New York, **1999**.

P163. Mechanistic Studies into Iron-Catalysed Alkene Isomerisation

Callum Woof
University of Bath, Bath, United Kingdom
Graduate Student
Advisor(s): Dr Ruth L Webster

https://twitter.com/Callum_Woof
@Callum_Woof

We have investigated the catalytic isomerisation of alkenes using a β-diketiminate iron(II) complex and a hydride source. Whilst we initially hypothesised this to be an entirely redox-neutral process in line with similar transformations,[1,2] upon studying the reaction further with a broad range of techniques including synthetic, EPR and electrochemical studies we now believe that the active species is an Fe(I) complex forming in situ, and the reaction proceeds by a redox-active pathway.

[1] M. Espinal-Viguri, R. L. Webster et.al., *Chem. Eur. J.*, **2016**, 22, 11605
[2] M. Espinal-Viguri, R. L. Webster et.al., *J. Am. Chem. Soc*, **2019**, 141, 572

P164. Rational design and synthesis of near-infrared phthalocyanine-based absorbing

Aymen Yaseen
Gebze Technical University, Kocaeli, Turkey
Graduate Student
Advisor(s): Ayse Gürek, Fabienne Dumoulin

https://twitter.com/AymenNYaseen
@AymenNYaseen

Photosensitizers for photodynamic therapy must ideally be excited by NIR wavelengths to reach deep-seated tumors.(1) Phthalocyanines are very suitable as their max. absorption can be tuned from 680 to 800 nm.(2,3) To benefit from the tumor-targeting Enhanced Permeation and Retention effect,(4,5) organosilica nanoparticles are aimed to be prepared from phthalocyanines absorbing at 800 nm. A careful design and synthetic strategy of appropriately functionalized phthalocyanines will be presented.

(1) Mallidi, S.; Anbil, S.; Bulin, A. L.; Obaid, G.; Ichikawa, M.; Hasan, T. Theranostics **2016**, 6 (13), 2458-2487.
(2) Lo, P. C.; Rodriguez-Morgade, M. S.; Pandey, R. K.; Ng, D. K. P.; Torres, T.; Dumoulin, F. *Chem. Soc. Rev.* **2020**, 49 (4), 1041-1056.
(3) Topal, S. Z.; Kumru, U.; Atilla, D.; Gürek, A. G.; Hirel, C.; Tommasino, J.-B.; Luneau, D.; Berber, S.; Dumoulin, F.; Ahsen, V. Dalt. Trans. **2014**, 43 (18), 6897-6908
(4) Maeda, H.; Nakamura, H.; Fang, J. Adv. Drug Deliv. Rev. **2013**, 65 (1), 71-79.
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P165. Synthesis of Nickel Nitrosyl Complexes with Bidentate N-heterocyclic Carbene Ligands

Zijie Zhang
Cal State Polytechnic University, Pomona, Pomona, United States
Undergraduate Student
Advisor(s): Dr. S. Chantal E. Stieber

https://twitter.com/zhang_zijie
@zhang_zijie

Activation of small molecules like NO offer insight towards biological reduction mechanisms. Nickel nitrosyl complexes were synthesized to examine the effect of NHC ligands on the nickel-NO bond. A new metal complex (MesNHC$_2$Me)Ni(COD) was synthesized and structurally characterized. A new Ni-NO complex [(MesNHC$_2$Me)Ni(NO)][BF$_4$] was synthesized and characterized by IR spectroscopy, which is a new example of a three-coordinate nickel nitrosyl complex with strongly sigma donating ligands.

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P166. Organotin(IV) Complexes as Catalyst for Biodiesel Formation: Synthesis, Structural Elucidation and Computational Studies

Muhammad Zubair
Quaid-i-azam university Islamabad, Islamabad, Pakistan
Graduate Student
Advisor(s):

https://twitter.com/zubairmarwatqau
@zubairmarwatqau

Here we have presented the synthesis of three novel triorganotin(IV) complexes. Spectroscopically characterized by NMR in solution and by FT-IR, X-ray diffraction analysis in solid state. The computational study was also performed. The homogeneous catalytic performance was evaluated for the transesterification of corn oil with methanol into biodiesel. The catalytic results revealed that the complexes are potential candidates for the development of new catalytic system for biodiesel production.

Muhammad Zubair. *Appl. Organomet. Chem.* **2020**, 34, e5305

Contact List

#	Name	Affiliation	Email	Twitter
P1	Stephen Aderinto	University of Sheffield	soaderinto1@sheffield.ac.uk	@AderintoStephen
P2	Jeanette Adjei	Western University	jadjei2@uwo.ca	@jeanette_adjei
P3	Mashael Alharbi	Cardiff University	alharbimm2@cardiff.ac.uk	@Mashaelmusaad
P4	Sk Amanullah	Indian Association for the Cultivation of Science	icsa2@iacs.res.in	@SkAmanullah
P5	Kori Andrea	Memorial University	kaandrea@mun.ca	@koriandrea
P6	Nayanthara Asok	York University	nynasok@yorku.ca	@NayantharaAsok
P7	Collen Bapiro	Midlands State University	bapirocollen@gmail.com	@firebapiro
P8	Zaira Barrera	University of California, Irvine	zbarrera@uci.edu	@zjbarrera
P9	Deepika Bedi	Texas Tech University	Deepika.bedi@ttu.edu	@deepika2705
P10	Roman Belli	University of Minnesota	rbelli@uvic.ca	@belli_roman
P11	Ali Ben Saida	University of Namur	ali.bensaida@unamur.be	@ali_bensaida
P12	Jordan Bentley	York University	bentleyj@yorku.ca	@BoronBentley
P13	Moulika Bhattacharyya	University of Windsor	mbhatt12@uwindsor.ca	@bhatt_mou
P14	Milan Bisai	CSIR-NCL Pune	mk.bisai@ncl.res.in	@BisaiMilan
P15	Hannah Bloomfield	University of Winnipeg	hannahrbloomfield@gmail.com	@slowlydiene
P16	Evan Bonnand	Cal State Polytechnic University, Pomona	efbonnand@cpp.edu	@Evan_Bonnand
P17	Andryj Borys	University of Edinburgh	andryjmborys@gmail.com	@AndryjBorys
P18	Sarah Boudreau	Cape Breton University	sarahboudreau10@gmail.com	@BoudreauChem
P19	Jamey Bower	Ohio State University	bower.214@osu.edu	@notJamey
P20	David Brossault	University of Cambridge	dffb2@cam.ac.uk	@BrossaultDavid
P21	Pavan C	Acharya and BM Reddy College of Pharmacy	pavan199864@gmail.com	@pavan_1998
P22	Rachele Carafa	Ryerson University	rachele.carafa@ryerson.ca	@rachcara23
P23	Jamie Carden	Cardiff University	CardenJL@cardiff.ac.uk	@jamie_carden
P24	Kurtis Carsch	Harvard University	kcarsch@g.harvard.edu	@kcarsch

P25	Cole Carter	Northwestern University	carterhcole@u.northwestern.edu	coal_carter
P26	Miguel Chacon Teran	Universidad Simon Bolivar (VE) / Universität Regensburg (DE)	mchacon233@gmail.com	@mchacon233
P27	Yukun Cheng	University of Minnesota	cheng715@umn.edu	@YukunCheng1
P28	Saurabh Chitnis	Dalhousie University	saurabh.chitnis@dal.ca	@chitnislab
P29	Marissa Clapson	University of Calgary	marissa.clapson@ucalgary.ca	@Chemrissa
P30	Omar Coughlin	Nottingham Trent University	omar.coughlin2017@my.ntu.ac.uk	@CoughlinOmar
P31	Gloria D'Amaral	Ryerson University	gloria.damaral@ryerson.ca	@gloriadamaral
P32	Cody Daneluik	Brock University	cd16qd@brocku.ca	@CodyDaneluik
P33	Pargol Daneshmandkashani	University of British Columbia	pargolkdaneshmand@gmail.com	@Pargol_D
P34	Johanna de Jong	Western University	jdejon7@uwo.ca	@JohdeJ
P35	Carlos Diaz	University of British Columbia	cdiazl@chem.ubc.ca	@_cdlz_
P36	Hai Dong	University of Michigan	haitdong@umich.edu	@haidong1301
P37	Liam Donnelly	University of Edinburgh	s1215530@sms.ed.ac.uk	@LiamDonChem
P38	Lorna Doyle	Trinity College Dublin	ldoyle8@tcd.ie	@ChemLorna
P39	Luis Duarte	University of Campinas	lg.alvesduarte@gmail.com	@lgalvesduarte
P40	Maeve Dufour	University of Windsor	dufou11c@uwindsor.ca	@maevedufour_11
P41	Gabriel Durin	French Alternative Energies and Atomic Energy Commission	gabriel.durin@cea.fr	@DurinGabriel
P42	Matthew Elsby	University of Ottawa	melsb080@uottawa.ca	@matthew_elsby
P43	Blaine Fiss	McGill University	blaine.fiss@mail.mcgill.ca	@Canuk_Chemist
P44	Amanda Fogh	University of British Columbia	mandyfogh@gmail.com	@mandyfogh
P45	Angelo Frei	University of Queensland	a.frei@imb.uq.edu.au	@Angelo_Frei
P46	Connor Frye	University of Minnesota	frye0048@umn.edu	@ConnorFrye42
P47	Mathieu Gama	University of Namur	mathieu.gama@unamur.be	@GamaMathieu
P48	NIDHI GARG	Ph.D.- IIT Kanpur	nidhigrg@iitk.ac.in	@Nidhigarg1994
P49	Lukas Gierlichs	Cardiff University	gierlichslj@cardiff.ac.uk	@LGierlichs
P50	Camilla Golec	Trent University	camillagolec@trentu.ca	@camillagolec
P51	Renée Goodman	University of Windsor	goodm111@uwindsor.ca	@ReneeBGoodman

P52	Chatura Goonesinghe	University of British Columbia	chaturad@chem.ubc.ca	@chaturad_g
P53	Matt Gray	Ohio State University	gray.1175@osu.edu	@Gray3311
P54	Megan Greaves	University of Strathclyde	megan.greaves@strath.ac.uk	@megangreaves7
P55	Marcus Grocott	University of Birmingham	mxg675@student.bham.ac.uk	@marcus_grocott
P56	Richa Gupta	National University of Singapore	e0267898@u.nus.edu	@gupta_richa1434
P57	Kriti Gupta	Indian Institute of Science Education and Research (IISER)	kriti.gupta@students.iiserpune.ac.in	@2342Kriti
P58	Dylan Hale	Dalhousie University	dylan.hale@dal.ca	@DylanHale1995
P59	Tyler Hannah	University of Calgary	tyler.hannah1@ucalgary.ca	@THannah77
P60	Alexander Harrison	University of Calgary	alexander.harrison@ucalgary.ca	@Alex_Harrison
P61	Brenda Henriquez	Cal State Polytechnic University, Pomona	bhenriquez@cpp.edu	@Brenda_H_2020
P62	Andrew Henry	Western University	ahenry48@uwo.ca	@AndrewHenryChem
P63	Angga Hermawan	Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University	angga.hermawan.r6@dc.tohoku.ac.jp	@anggahermaw
P64	Gabriele Hierlmeier	University of Regensburg	Gabriele.hierlmeier@ur.de	@GHierlmeier
P65	Alexis Hoxie	Cal State Polytechnic University, Pomona	ashoxie@cpp.edu	@alexis_chem
P66	Vineet Jakhar	University of Florida	vjakhar@ufl.edu	@jakhar_vineet
P67	Hyuk-Joon Jung	University of British Columbia	hyukjoon@chem.ubc.ca	@Chem_Joon
P68	Vishal Kachwal	(BITS Pilani, Pilani campus) Birla Institute of Technology and Science	p2014015@pilani.bits-pilani.ac.in	@kachwal_vishal
P69	Johannes Karges	University of California, San Diego	jkarges@ucsd.edu	@Johannes_Karges
P70	Jaspreet Kaur	PCTE group of institute ludhiana	jaspreetsidhu885@gmail.com	@jaspree75604402
P71	John Kelly	University of Regensburg	john.kelly@ur.de	@TheWolf_Group
P72	Samim Khan	Aliah University	samimchm@gmail.com	@samim_2k
P73	Mohammad Shahnawaz Khan	Aligarh Muslim University	khanshahnawazamu@gmail.com	@Sarcastickhan1

P74	Diana Kim	University of British Columbia	ddhkim@chem.ubc.ca	@Diana_Chem
P75	Marcus Kindervater Kindervater	Dalhousie University	mr454450@dal.ca	@mbkindervater
P76	Ross Koby	Vanderbilt University	ross.f.koby@vanderbilt.edu	@rawssk0be
P77	Natalie Korkola	Western University	nkorkola@uwo.ca	@NatalieKorkola
P78	Errikos Kounalis	Utrecht University	errikoskounalis@hotmail.com	@ErrikosKounalis
P79	Daniel Kowalski	University of Glasgow	d.kowalski.1@research.gla.ac.uk	@dankowalskichm
P80	Kelsie Krantz	University of Virginia	kek6nc@virginia.edu	@kek_kelsie
P81	Viveka Kulkarni	Mount Allison University	vkkulkarni@mta.ca	@KulkarniViveka
P82	Jonathan Kuo	University of Pennsylvania	jonlkuo@sas.upenn.edu	jonathanlkuo
P83	Jan-Willem Lamberink	Western University	jlambe23@uwo.ca	@JwLamberink
P84	Michael Land	Carleton University	michael.land@carleton.ca	@MikeL4nd
P85	Andres Lara Contreras	Department of Chemistry and Chemical Engineering - Royal Military College of Canada	laracontreras1295@gmail.com	@AndresLaraCo
P86	Nadia Laschuk	Ontario Tech University	nadia.laschuk@ontariotechu.net	@laschuk_
P87	Dominique Leckie	University of Windsor	leckied@uwindsor.ca	@ladominiquee
P88	Julia Leitl	Institute of Inorganic Chemistry, University of Regensburg	julia.leitl@ur.de	@julia_leitl
P89	Tyra Lewis	Department of Forensic Science, Environmental and Life Sciences, Trent University	tyralewis@trentu.ca	@siwelaryt
P90	Qiuming Liang	University of Toronto	walter.liang@mail.utoronto.ca	@WalterQLiang
P91	Jun Yang Liu	University of Windsor	liu1be@uwindsor.ca	@ljyangjun
P92	Kaitlynn Lopes	Boston University	kmlopes@bu.edu	@klvettegirl715
P93	Bruno Luppi	University of Alberta	luppi@ualberta.ca	@luppi_bruno
P94	Casper Macaulay	Dalhousie University	casper.macaulay@gmail.com	@eTheR_ealCasper
P95	Damien Mahaut	University of Namur	damien.mahaut@unamur.be	@DMahautChem
P96	Aleena Malik	Univeristy of Windsor	malik12m@uwindsor.ca	@amalik283
P97	Basel Mansour	University of Windsor	manso11h@uwindsor.ca	@BaselMa42697042

P98	Kate Marczenko	Dalhousie University	kt991187@dal.ca	@KMMarczenko
P99	Gage Mason	University of Windsor	mason114@uwindsor.ca	@magegason
P100	Kathleen May	Ryerson Univeristy	kathleen.may@ryerson.ca	@khem4may
P101	Ryan McGuire	Dalhousie University	ryan.mcguire@dal.ca	@_mcguireryan
P102	Paul Meister	University of Windsor	meisterp@uwindsor.ca	@meisterp3
P103	Adyn Melenbacher	Western University	amelenba@uwo.ca	@adynmelenbacher
P104	Maximilian Menche	Catalysis Research Laboratory (CaRLa)	maximilian.menche@carla-hd.de	@maxmenche
P105	AB MIR	IIT Gandhinagar	ab.qayoom@iitgn.ac.in	@mir_qayoom
P106	Rajarshi Mondal	University of Manitoba	rajarshi.juchem@gmail.com	@JuchemMondal
P107	Madison Mooney	University of Windsor	moone114@uwindsor.ca	@Madison77772905
P108	Patrick Morgan	University of Nottingham	patrick.morgan@nottingham.ac.uk	@azure_wanderer
P109	Alexandra Nagelski	Yale University	a.nagelski@yale.edu	@ANagelski
P110	Mitchell Nascimento	University of Victoria	nascime@uwindsor.ca	@MitchellNas
P111	Chris Nicholas	Honeywell UOP	christopher.nicholas@uop.com	@CatalysisChris
P112	Pranay Ninawe	Indian Institute of Science Education and Research, Pune, India	pranay.ninawe@students.iiserpune.ac.in	@000pranay
P113	Lucie Nurdin	University of Calgary	lucie.nurdin@ucalgary.ca	@lucie_nurdin
P114	Kudzanai Nyamayaro	University of British Columbia	knyamayaro@chem.ubc.ca	@KudziNyamayaro
P115	Audithya Nyayachavadi	University of Windsor	nyayacha@uwindsor.ca	@anyayach
P116	Meagan Oakley	University of Minnesota	moakley@umn.edu	@meaganoakley
P117	Michael Ocheje	University of Windsor	ochejem@uwindsor.ca	michocheje
P118	Elisa Olivas	Cal State Polytechnic University	emolivas@cpp.edu	@ElisaOlivas4
P119	Robert Ortiz	University of Manitoba	ortizr@myumanitoba.ca	@OrtizRobert44
P120	Arnaud Osi	UNamur	arnaud.osi@unamur.be	@ArnaudOsi
P121	Darren Ould	Cardiff University	dmo33@cam.ac.uk	@darren_ould
P122	Sanjukta Pahar	CSIR-National Chemical Laboratory	sanjuktaapahar@gmail.com	@PaharSanjukta

P123	Nabhendu Pal	Indian association for the cultivation of science	nabhendu92@gmail.com	@nabhendupal
P124	Joseph Palomba	UC San Diego	jpalomba@ucsd.edu	@PeriodiKangeroo
P125	Gemma Parker	University of Warwick	g.parker.3@warwick.ac.uk	@GemmaParker0110
P126	Löwe Pawel	Westfälische Wilhelms-Universität Munster	p.loewe@uni-muenster.de	@PawelLoewe
P127	John Pham	Colgate University	jpham@colgate.edu	@jjrpham
P128	Ariprasanth Ramalingam	SRM University	ariprasanth.r@gmail.com	Ariprasanth 4
P129	Ravindra Raut	Indian Institute of Science Education and Research, Pune	ravindra.raut@students.iiserpune.ac.in	@ravindraraut19
P130	Hootan Roshandel	University of British Columbia	hootanr@chem.ubc.ca	@hootan_r
P131	Anupom Roy	University of Windsor	roy11k@uwindsor.ca	@Anupom88
P132	Sourav Roy	Indian Institute of Science	sr8kol@gmail.com	@souravscott
P133	Mira Rupp	Université de Montréal, Universitaet Wuerzburg	mira.rupp@umontreal.ca	@MiraRupp
P134	Artemis Saddington	University of Oxford	artemis.saddington@sjc.ox.ac.uk	@artemis_sadd
P135	Sabrina Scott	University of British Columbia	sscott@chem.ubc.ca	@sabselscott
P136	Anmol Sharma	University of the Fraser Valley	anmol.sharma@student.ufv.ca	@anmol98z
P137	Natali Shevchenko	Université de Montréal	nrshevchenko@gmail.com	@NataliShevche15
P138	Jan-Erik Siewert	LIKAT Rostock	jan-erik.siewert@catalysis.de	@siewert_jan
P139	Aniela Silva Nolasco	Universidad JuÃ¡rez AutÃ³noma de Tabasco	animonsino@gmail.com	@anni_nolasco
P140	Kaitlyn Silverthorne	Ryerson University	kaitlyn.silverthorne@ryerson.ca	@silverthornekt
P141	Arpita Singh	Texas Tech University	arpita.singh@ttu.edu	@Arpita1391
P142	Kathleen Snook	Boston University	kmsnook@uw.edu	asexualchemist1
P143	Miguel Soto	University of British Columbia	msoto@chem.ubc.ca	@Miguel_A_Soto_
P144	Anandi Srinivasan	Laboratoire d'Electrochimie Moléculaire LEM, Paris	anandi.srinivasan@u-paris.fr	@AnandiSrinivas1
P145	Blake St. Onge	University of Windsor	stongep@uwindsor.ca	@Stonge912

P146	Alexander Stöckli	Mount Allison University	ahstockli@mta.ca	@HubertStockli
P147	Katarina Stefkova	Cardiff University	StefkovaK@cardiff.ac.uk	@KatarinaStefko1
P148	S. Maryamdokht Taimoory Taimoory	University of Michigan, Chemistry Department	seyedeht@umich.edu	@NTaimoory
P149	Kaeden Teindl	University of the Fraser Valley	kaeden.teindl@student.ufv.ca	@KTeindl
P150	Shailabh Tewari	Indian Institute of Technology, Delhi	shailabh.tewari@gmail.com	@ShailabhTewari
P151	Gilian Thomas	University of Victoria	gilian.t.thomas@gmail.com	@gilian_thomas
P152	Richard Thompson	Louisiana State University	rrthompson@lsu.edu	@RichardRThomps1
P153	Adrian Torres	Cal State Polytechnic University, Pomona	adriant1@cpp.edu	@AdrianChem
P154	Carlos Torres-Méndez	Escuela de Quimica, Facultad de Ciencias QuÃimicas y Farmacia, Universidad de San Carlos de Guatemala	caarce94entropy@gmail.com	@randomrandom901
P155	Jonah Toth	University of Toronto	jonah.toth@mail.utoronto.ca	@jonahtoth
P156	Warren VandeVen	University of the Fraser Valley	wrvwarren@gmail.com	@VandevenWarren
P157	Gloria Vigueras	University of Murcia	gloria.vigueras@um.es	@ViguerasGloria
P158	Henry Walsgrove	University of British Columbia	henryw@chem.ubc.ca	@HWalsgrove
P159	JinZhao Wang	McMaster University	wangjz2@mcmaster.ca	@zoomjin19
P160	Lara Watanabe	University of Windsor	watanabl@uwindsor.ca	@larawatanabe
P161	Athi Welsh	Chemistry	wlsath001@myuct.ac.za	@athiwelsh
P162	Lucienna Wolf	DePaul University	luciennawolf@gmail.com	@LucyWol58238133
P163	Callum Woof	University of Bath	c.woof@bath.ac.uk	@Callum_Woof
P164	Aymen Yaseen	Gebze Technical University	anyaseen@gtu.edu.tr	@AymenNYaseen
P165	Zijie Zhang	Cal State Polytechnic University, Pomona	zijiezhang@cpp.edu	@zhang_zijie
P166	Muhammad Zubair	Quaid-i-azam university Islamabad	mzubair@chem.qau.edu.pk	@zubairmarwatqau