



CHEMISTRY

UNDERGRADUATE
RESEARCH CONFERENCE

2 APRIL 2015
12:30 - 3:30 PM

IRVING K BARBER LEARNING CENTRE
DODSON ROOM

12:30 - 12:35		Opening remarks
12:35 - 12:55	Loryn Arnett	Development of Novel Chiral Nematic Materials via Templating with Cellulose Nanocrystals
12:55 - 13:15	Jay Chi	Titanium Catalyzed Synthesis of Amines
13:15 - 13:35	Benjamin Boswell	Construction of Key Fragment of Mandelalide A via Radical Cyclization Methodology
13:35 - 13:55	Caroline Pao	Computational Studies of Transition Metal-doped Single-Walled Carbon Nanotubes (SWNTs)
13:55 - 14:05		Coffee break
14:05 - 14:25	Paniz Pahlavanlu	Novel Bridged Polyacenes for Solar Cell Applications
14:25 - 14:45	Madeleine lafrate	Lanthanide Complexes for the Treatment of Osteoporosis
14:45 - 15:05	Alex Gatien	Synthesis of N,O-chelated Tungsten Alkylidenes and their reactivity towards Olefin Metathesis
15:05 - 15:25	Hojung Lee	Cyclization of Natural Products via Iodonium Salts
15:25 - 15:30		Closing remarks

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PARTICIPATING PRESENTERS

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presentations to the audience

Cyclization of Natural Products via Iodonium Salts

Hojung Lee | 3:05 PM

Hypervalent iodine species are of great importance in synthetic chemistry. One such example would be the widely known λ^5 oxidant: Dess-Martin periodinane, which is a versatile reagent converting alcohols to aldehydes and ketones. In recent years, λ^3 iodonium salts have been promising candidates for replacing metal catalysts such as Pd, Pb, Tl, Hg due to their stable nature and low toxicity. In particular, the ability for iodonium salts to undergo reductive elimination, which is a common feature of transition metal complexes, proves to be useful for applications such as cross-coupling reactions, arylation of heteroatoms, and C-H activation. My research project is to utilize the electron-deficient nature of the diaryliodonium salts to test whether they can assist in cyclization of aliphatic carbon chains, and the possibility of undergoing cascade reaction with poly-olefin systems to form multiply fused rings.

Development of Novel Chiral Nematic Materials via Templating with Cellulose Nanocrystals

Loryn Arnett | 12:35 PM

Cellulose nanocrystals (CNCs) are derived from bulk cellulose, an abundant polymer found in plants and trees. This renewable material behaves as a liquid crystal in aqueous solution, forming chiral nematic layers. These are photonic, in that they reflect circularly polarized light with λ_{max} dependent on the helical pitch and observation angle. It has been shown previously that self-assembly of CNCs can be exploited to template silica and organosilica precursors, resulting in chiral nematic mesoporous organosilica films after template removal. Imposing chirality into mesoporous silica materials has applications in chiral chromatography or catalysis, while its photonic properties may allow them to function as sensors. This synthetic strategy has been expanded here to incorporate highly hydrophobic organosilane precursors, including hexylene and biphenyl-bridged species by manipulation of solvent composition. The use of these mesoporous organosilica films to hard-template polymerized C_{60} is also investigated.

Titanium Catalyzed Synthesis of Amines

Jay Chi | 12:55 PM

Amines are essential functional building blocks in a variety of natural products in the pharmaceutical, agrochemical, and fine chemical industries. Classical approaches to amine preparation include direct N-alkylation with alkyl halides, reductive amination of carbonyl compounds, and reduction of nitro compounds. Hydroamination and hydroaminoalkylation are two catalytic approaches to synthesize amines in an atom-economic fashion. If achieved

selectively, it offers a facile method to make amine substrates, which can be then made into more complex products. Titanium, a group IV transition metal, is earth-abundant, relatively inexpensive, and less toxic in comparison to many other metals. The reactivity of three titanium complexes bearing tethered aryl oxide ligands are investigated for their capacity to catalyze intramolecular hydroamination. Furthermore, bis(pyridonate)bis(dimethylamido) titanium systems are investigated for hydroaminoalkylation experimentally, as well as using Gaussian computationally.

Construction of Key Fragment of Mandelalide A via Radical Cyclization Methodology

Benjamin Boswell | 1:15 PM

At a depth of 18 m off a reef in South Africa, hidden in a sea sponge, a rare family of four glycosylated polyketide macrolides called the Mandelalides (the namesake being Mandela) were surfaced last year. One in particular, Mandelalide A, displayed exciting cytotoxicity against human NCI-H460 lung cancer cells ($IC_{50} = 12$ nM) and mouse Neuro-2A neuroblastoma cells ($IC_{50} = 29$ nM). An efficient chemo-synthesis of these highly complex and stereospecific macrolides is crucial for further cellular assays and medicinal chemistry exploration. Mandelalide A has been synthesized before, however, this work explores a new approach to the synthesis utilizing a key tandem, stereoselective radical cyclization that displays not only potential for a more rapid assembly than previous efforts, but would also allow for adaptation to the synthesis of the remaining Mandelalide kin.

osteoporosis. The focus of my project has been to expand upon the current library of bifunctional chelators for lanthanum within the Orvig group, as well as devising some physical tests to establish whether binding of the complex to HAP can be detected *in vitro*.

Synthesis of *N,O*-chelated Tungsten Alkylidenes and their Reactivity Towards Olefin Metathesis

Alex Gatien | 2:45 PM

Olefin metathesis involves the redistribution of alkene fragments to afford new olefinic products using metal-carbon multiply bonded complexes. This catalytically mediated process has important applications for pharmaceuticals, polymers and natural product synthesis, enabling reactivity which has traditionally been challenging or inaccessible. Group 6 alkylidene complexes have shown to be highly active for these transformations. The Schafer group has successfully used *N,O*-chelating ligands for a range of catalytic transformations, with the binding modes and hemilability of these ligands rendering them highly useful. To date, no known *N,O*-chelated tungsten alkylidenes exist in the literature and their reactivity towards olefin metathesis is unknown. Thus, *N,O*-chelated tungsten alkylidene complexes were synthesized, characterized and their reactivity towards cross metathesis, ring opening metathesis polymerization and ring closing metathesis were explored.

Novel Bridged Polyacenes for Solar Cell Applications

Paniz Pahlavanlu | 2:05 PM

The Shockley–Queisser limit of 33% has limited traditional routes to more efficient solar cells. However by incorporating materials capable of undergoing singlet fission, a process in which a singlet excited chromophore interacts with an adjacent chromophore to produce two triplet excited states, solar cell efficiencies of 50% may be reached. While singlet fission in polyacenes has received considerable attention, the bulk of this research has focused on highly crystalline structures. To investigate the scope of singlet fission, covalent coupling of polyacenes is desired. In particular, the incorporation of a sulphur bridge between two polyacenes would allow tuning of optical properties through facile oxidation of the bridge. The synthesis and optical characterization of sulphur-bridged anthracenes will be discussed in the context of singlet fission applications.

Lanthanide Complexes for the Treatment of Osteoporosis

Madeleine lafrate | 2:25 PM

The f-elements have high affinity for the inorganic hydroxyapatite (HAP) matrix that constitutes 90% of the skeleton. Lanthanides (including lanthanum) usually form stable trivalent ions in aqueous solutions, and this is very useful in the current medicinal applications of lanthanides, which include MRI contrast agents and phosphate binding agents. One phosphate-binding agent in particular, lanthanum carbonate (Fosrenol®), was shown to positively impact bone mineral density (BMD) in ovariectomized rats, thus forming an interesting new basis for research in drugs to treat BMD disorders such as

Computational Studies of Transition Metal-doped Single-Walled Carbon Nanotubes (SWNTs)

Caroline Pao | 1:35 PM

Owing to their unique mechanical and electrical properties, carbon nanotubes (CNTs) have numerous prominent applications, including chemical sensors, nanobioelectronics, and hydrogen storage. The electrical properties can be manipulated through either functionalization or doping. Past research has investigated the external doping of transition metal atoms into the supramolecular carbon framework and suggested a resulting higher conductivity and reactivity of the system. However, the internal doping of CNTs has not yet been studied but is of great interest due to the predicted reactivity differences on the internal face of the nanotubes. Thus, this project studies the exo- and endo-doping of nickel into single-walled CNTs (SWCNTs) and the resulting energy gap using density functional theory to provide some theoretical guidance in this important field. Chiral SWCNTs are heavily emphasized due to the strong electrical dependence of the nanotubes on chirality. Moreover, since the computational costs increase dramatically with the size of the nanotube systems, the most accurate theories are far beyond affordable, even with the rapid growth of computing resources. Therefore, this project includes the search for suitable approximation models to allow for the study of large CNT systems at low computational costs.

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