

ABSTRACTS

Undergraduate Research in Chemistry Regional Poster Competition

Jacobs Science Building

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Department of Chemistry
University of Kentucky
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DIFFERENTIATION OF ISOMERIC HEPARAN SULFATE USING MASS SPECTROMETRY, TANDEM MASS SPECTROMETRY AND PRINCIPLE COMPONENT ANALYSIS.

John Attelah, Junior, Chemistry, Berea College

Isaac Agyekum, Chemistry, The University of Georgia

Glycosaminoglycans (GAGs) are complex polysaccharides, expressed at the cell surface and in the extra-cellular matrix, which comprise the carbohydrates portion of proteoglycans and are found in a variety of organisms ranging from bacteria to humans. GAGs participate in a number of significant biological processes, such as cell-cell and cell-matrix signaling at the origin of a variety of physiological and pathological functions such as embryonic development, cell adhesion, the regulation of biochemical pathways, cell growth and differentiation, homeostasis, and the mediation of inflammatory reactions. They have also been implicated in the initial step of some pathogenic infections and have been observed to undergo some alteration in some tumor growth. There are different types of GAGs which include Chondroitin Sulfates(CS), Dermatan Sulfates(DS), Keratan Sulfates(KS), Heparin and Heparan Sulfates(HS). Since a better understanding of structural, and binding properties of HS is required for development of HS mimetic, and possible new glycotherapeutics, increasing interest in protein-carbohydrate interactions is accompanied by challenging demand for viable, accurate and high-throughput methodology for their characterization. Therefore, the objective of the project was to use Mass spectrometry, Fourier Transform Mass Spectrometry and Principal Component Analysis (PCA) to diagnostically distinguish between isomeric Heparan Sulfate Glycosaminoglycans.

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A COMPARISON OF TWO BLOOD SERUM MOLECULES AND CEREBRAL BLOOD FLOW IN AD PATIENTS

Max Baker, Senior, Chemistry, University of Kentucky

Alzheimer's disease is the most common form of dementia in the United States and is the sixth leading cause of death. One of the most challenging components of the disease is being able to determine if certain proteins, enzymes, lipids, and other molecules at varying levels influence the development of the disease. The purpose of this study was to determine if there is a correlation between certain blood serum molecules and cerebral blood flow obtained from brain imaging in humans. Specifically, Prostaglandin-D-Synthase (PTGDS) and Transthyretin (TTR) levels will be measured from the blood and compared to brain images. PTGDS is an enzyme that catalyzes the isomerization of Prostaglandin-H₂ to Prostaglandin-D₂, and further acts as a major protein in human cerebrospinal fluid as a ligand-binding protein as it has high affinities for retinoids, thyroids, and bile pigments. This molecule helps induce sleep, is critical in the development of allergic diseases such as asthma, and acts as a precursor for a series of prostanoids. Transthyretin is a carrier protein that carries thyroid hormones in the plasma and cerebrospinal fluid and retinol in the plasma. It is secreted into the cerebrospinal fluid by the choroid plexus and it has been shown that misfolding and aggregation of TTR can lead to a variety of amyloid diseases.

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AMMUNITION DIFFERENTIATION BY ICP-AES ANALYSIS OF GUNSHOT RESIDUE

Chris Barbera, Senior, Chemistry, Hanover College

Craig Philipp, Chemistry, Hanover College

Most gunshot residue, or GSR, testing is a simple positive or negative response to the presence of GSR. There are not many techniques that easily give qualitative and quantitative data of GSR limiting the information that can be used. We used ICP-OES in an attempt to quantify four elements in different brands of ammunition. Seven brands of ammunition were differentiated using ICP-OES to quantify and find ratios of seven elements commonly found in GSR. The ammunition was all fired from the same gun and was thus of similar type. The data was collected from freshly fired ammunition, and prepared for measurement on ICP-OES by dissolving the residue in nitric acid. Ratios and ranges of Fe:Ba:Pb:Zn:Mg:Al:K, with iron set to one were created for each of the seven different brands of ammunition. The seven brands were found to have statistically relevant differences (95% certainty) in the Fe:Ba:Pb:Zn:Mg:Al:K ratio. In addition, we are testing gunshot residue left on the hand of a person shooting the gun to determine whether we can tell the type of ammunition used by the above ratios. Ideally, this technique could be applied in a criminal forensic laboratory setting as an evidence processing method that could aid investigations.

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INVESTIGATING THE IN SILICO OPTICAL CHARACTERISTICS OF TRIALKYLSILYLETHYNYL PENTACENE DERIVATIVES USING GW-BSE CALCULATIONS

Kristen Brooks, Senior, Chemistry, University of Kentucky

Karol Jarolimek, Chemistry, University of Kentucky

Chad Risko, Chemistry, University of Kentucky

Solar cells convert energy from light into electricity via the photovoltaic effect. The theoretical power conversion efficiency of conventional inorganic solar cells using a p-n junction is limited by the Shockley-Queisser Efficiency Limit; however, organic semiconductors which utilize singlet fission have been found to exceed this limit. Two such organic semiconductors are 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS pentacene) and 6,13-bis(triethylsilylethynyl) pentacene (TES pentacene), which respectively adopt two-dimensional brickwork and one-dimensional slipped-stack packing arrangements. Despite similarities in the structures of these two molecules, their performances as organic semiconductors vary significantly as a result of their packing arrangements. In this experiment, the in silico optical characteristics of brickwork and slipped-stack polymorphs of both TIPS pentacene and TES pentacene were calculated using GW approximations coupled with BSE (Bethe-Salpeter Equation). By comparing these optical characteristics, the effects of packing arrangement on organic solar cell performance may be further determined.

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EFFECTS OF SURFACE MODIFICATION ON THE PHOTOLUMINESCENCE QUANTUM YIELD OF METHYLAMMONIUM LEAD IODIDE PEROVSKITES

Jillian Cramer, Senior, Chemistry, University of Kentucky

Kenneth Graham, Chemistry, University of Kentucky

Methylammonium lead iodide perovskites have been shown to be an effective light-absorbing active layer in solar cells, but suffer from low stability and inconsistent performance due in part to defects at the surface. These defects can lead to “trap states,” inhibiting the transport of charge carriers across the device and increasing unwanted nonradiative decay. However, surface modifiers, such as phosphonic acids, carboxylic acids, thiols, trichlorosilanes, amines, and zwitterions studied here, may improve the surface chemistry and mitigate the formation of trap states. Ideally, the surface modifiers strongly bind to the lead iodide perovskite and improve the performance and stability of the cells. In this work we test the hypothesis that these surface modifiers will positively effect the radiative emission via photoluminescence, suggesting the reduction of trap states within the perovskite films and improved performance as a photovoltaic material.

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NITROGEN DOPED CARBON NANO-ONIONS AS ELECTROCATALYSTS FOR OXYGEN REDUCTION REACTIONS

Nicholas Demas, Senior, Chemistry, University of Kentucky

Yan Zhang, Chemistry, University of Kentucky

Oxygen reduction reaction (ORR) can occur via two pathways. One pathway is a four-electron process in which oxygen is converted into water, which is a highly desirable reaction for efficient low-temperature energy conversion devices. In these devices, hydrogen is oxidized at the anode and oxygen is reduced at the cathode. Platinum and platinum-based alloys are the current catalysts for ORR in these devices. However, these catalysts are expensive, have long-term stability issues, and become incredibly inefficient over time. Nitrogen doped carbon nano-onions (n-CNOs) are a promising alternative to the current electrocatalysts used for oxygen reduction reactions. Modified carbon materials have already been shown to have excellent electrocatalytic activity, but this research focuses on the incorporation of nitrogen into the carbon nano-onion microstructure. These n-CNOs have onion-like structures have high surface areas with many active sites for ion adsorption to allow for fast electron transfer kinetics at the electrocatalyst surface. The electrocatalytic activity of n-CNOs was assessed using both a rotating disk electrode and ring rotation disk electrode. This research is important for the advancement of energy conversion devices, as many of the current electrocatalysts used have long-term problems that may render these devices obsolete. The results showed that n-CNOs have excellent electrocatalytic performance qualities and better long-term stability and efficiency, making them a possible replacement for the current platinum-based electrocatalysts.

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KINETIC INVESTIGATION OF RING-OPENING POLYMERIZATIONS USING A BIMETALLIC CATALYST

Benjamin Demor, Senior, Chemistry and Biochemistry,

Rose-Hulman Institute of Technology

Stephanie Poland, Chemistry and Biochemistry, Rose-Hulman Institute of Technology

Research on biodegradable polymers is of interest as they have many applications in the biomedical field. Two such polymers that can be used for these applications are poly(trimethylene carbonate) and polylactide. In this study, a previously developed and investigated bimetallic magnesium catalyst was used for a catalytic ring-opening polymerization (ROP) of trimethylene carbonate (TMC) and lactide. A kinetic investigation using IR spectroscopy and an attempt at ^1H NMR spectroscopy found that the catalyzed reaction occurs at a faster rate than previously believed. With the use of ^1H NMR to monitor reaction conversion, it was shown that the ROP of lactide with this catalyst is inefficient with very long reaction times. The development of these kinetic investigations for the two cyclic monomers will be discussed.

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1-exo-AcAP: TOTAL SYNTHESIS AND IT'S CRYSTALLIZATION

Weixia Deng, Senior, Chemistry, University of Kentucky

Loline species are potent insecticidal agents produced by endophytic fungi of cool-season grasses. Loline is a saturated 1-exo-aminopyrrolizidine with an oxygen bridge between carbons 2 and 7. In my independent research, the study object is (\pm)-1-exo-acetamidopyrrolizidine (exo-AcAP), which is the biosynthetic precursor of N-acetylnorloline.

The purpose of this project is to synthesize exo-AcAP and then do some research on exo-AcAP crystallization. My synthesis scheme contains seven steps starting with L-proline. The methodology of exo-AcAP synthesis was developed by Minakshi Bhardwaj. The (exo-AcAP) $_2$ ·HCl complex salt was recently discovered by Bhardwaj when she was trying to crystallize exo-AcAP in chloroform; the source of HCl was the slow decomposition of CHCl $_3$. This dimer salt contains a bonding interaction like $\equiv\text{N}-\text{H}^+-\text{N}\equiv$. Some unpublished results suggest that the "proton bridge" bond is abnormally short, and this kind of 2:1 ratio salt is very rare. In order to have a better study to the dimer salt, I dissolved exo-AcAP into CDCl $_3$ and attempt to crystallize it to obtain (exo-AcAP) $_2$ ·DCl salt. There also have one potential variable could relate to the formation of dimer salt, which is the rate of HCl addition. In this case, I will present a salt formation and crystallization by letting the free base directly react with HCl gas.

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THE SYNTHESIS AND SPECTROSCOPY OF NINE BENZIL-BASED LIGANDS AND THEIR PALLADIUM (II) COMPLEXES

Eric Dobias, Sophomore, Chemistry, Thomas More College

Tyler Green, Chemistry, Thomas More College

Daniel Esterline, Chemistry, Thomas More College

Diimine ligands have various uses in pharmaceuticals, industry, and major biological processes. The purpose of this research was to synthesize the ligands N,N'-di(4-bromophenyl)-1,2-diphenylethane-1,2-diimine and N,N'-di(4-methoxyphenyl)-1,2-diphenylethane-1,2-diimine as well as six analogues using different aniline reagents. The aniline compounds contain different substituents in varied positions on the benzene ring, which may impact the overall viability of the reactions. Benzil and toluene-sulfonic acid were reacted with the appropriate aniline starting material. The products have been characterized by ¹H NMR Spectroscopy, Infrared Spectroscopy, and Gas Chromatography Mass Spectrometry. Results indicate that the original two ligands were successfully synthesized with 65-75% yields, while the p-nitroaniline and m-nitroaniline ligands were not formed/recovered. Future work includes the synthesis and purification of further analogues as well as complexation with palladium and lead.

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EXPERIMENTAL DESIGN OF RING OPENING POLYMERIZATION OF CYCLOHEXENE OXIDE BY SOLID CO₂

Taylor Downs, Senior, Chemistry, Rose-Hulman Institute of Technology
Dr. Stephanie Poland, Chemistry, Rose-Hulman Institute of Technology

Carbon dioxide and epoxide coupling to yield polycarbonates has been a major focus in plastics research since its discovery in 1969 by Shohei Inoue. The downfalls to using this original method in undergraduate laboratories involve unsafe reaction conditions because of the high pressures of CO₂ required and the need for costly stainless steel reactors. Many advancements towards making this synthesize less hazardous include using ambient reaction temperatures, operating at 1 atm pressures in the reaction vessels, and utilizing less reactive epoxides. All these changes lead to the greener synthesis of polycarbonates that can be used in electronics, consumable goods, optical media, and the automotive and medical industries. This study focuses on creating a laboratory experimental design to introduce undergraduate students to catalysis, polymerization, and green chemistry. Using techniques used in a previous Organic Chemistry lab at RHIT, carbon dioxide and air-stable cyclohexene oxide were coupled using various transition metal catalysts and cocatalysts in a plastic centrifuge tube. The products were analyzed using ¹H NMR as well as FT-IR spectroscopy. Three (salen)MCl catalysts (M = Co³⁺, Al³⁺, Cr³⁺) were studied to determine which catalyst showed the highest coupling activity. This seminar will detail the optimization route taken toward the goal of successfully producing poly(cyclohexene carbonate) under these restricted conditions.

A COMPARISON OF DIGESTION METHODS FOR THE ANALYSIS OF HUMAN CREMATED REMAINS**Christina Farwick, Senior, Chemistry, Thomas More College**William Wetzel, Chemistry, Thomas More College

Over a decade ago, the owner of the Tri-State Crematory in Noble, GA was prosecuted for the improper disposal of deceased human bodies. Through investigation, the authorities discovered that families were given cement powder in place of their loved one's ashes. Because authentic human cremated remains are visually indistinguishable from a variety of other materials, many studies have examined instrumental methods for determining the validity of supposed human ashes. In this work, two different microwave reaction vessels, GlassChem and EasyPrep Plus, and sets of digestion parameters were evaluated for the preparation of genuine human cremated remains and various other physically-similar solids (cement, grout, dirt, sand, fertilizer, vermiculite, fireplace ash, gravel, and animal remains). Inductively Coupled Plasma-Atomic Emission Spectrometry was subsequently used to determine the trace metal levels. Elements displaying the most variation across all samples were plotted two-dimensionally to distinguish authentic human cremated remains from other materials. This method was successful to a certain degree; however, a principal component analysis of the trace metal data more clearly classified the samples. Finally, the two microwave digestion methods were compared to determine if one was more effective at distinguishing cremains from non-cremains.

SYNTHESIS OF BENZO[b][1,4]THIAZINE-6-CARBOXAMIDE DERIVATIVES AS NOVEL ANTI-EPILEPTIC AGENTS**Abigail Florence, Senior, Chemistry, University of Kentucky**Adam McCluskey, Chemistry, University of Newcastle, AustraliaAndrew Lin, Chemistry, University of Newcastle, Australia

Epilepsy is a neurological disorder that results in frequent seizures, which can lead to a poor quality of life. This disease occurs due to the rapid release, via exocytosis, of neurotransmitter within the brain. It is believed that by being able to slow down the number of vesicles each neuron recycles, the number of seizures within an individual can be reduced or eliminated. A screening of a library of 17,000 compounds showed that benzo[b]thiazine-6-carboximide 1 displayed anti-epileptic activity. A library of compounds was synthesized to establish the exact structure to activity (SAR) relationship of the original compound to the protein interactions. The first key reaction made up the first library of compounds and involved the Knoevenagel condensation, which reacts aldehydes and ketones together in the presence of a weak base. The second key reaction was N-alkylation, which binds an aliphatic amine with a secondary alkyl halide to make up the second library of compounds. The third, and final, reaction was amide coupling, which binds a carboxylic acid with an amine to make up the final library of compounds. All of the compounds for each library have been synthesized and are awaiting an evaluation of biological activity at both Children's Medical Research Institute in Sydney, Australia and Calvary Mater Hospital in Newcastle, Australia.

ALGAE-MEDIATED CONVERSION OF CO₂ EMISSIONS TO DIESEL-RANGE HYDROCARBONS**Erin Molly Frazar, Senior, Chemical Engineering, University of Kentucky**Robert Pace, Chemistry, University of KentuckyRyan Loe, Chemistry, University of KentuckyEduardo Santillan-Jimenez, Chemistry, University of KentuckyMark Crocker, Chemistry, University of Kentucky

Algae-based carbon capture provides a multifaceted solution to the issue of rising greenhouse gas levels. Direct reduction of CO₂ gas emissions as well as utilization of valuable algae components are some of the benefits realized through this approach. However, the overall efficiency and economic constraints of algal processing and upgrading present challenges that prevent microalgae from becoming a viable fuel source. The proposed work is designed to optimize algal lipid extraction and purification processes in order to avoid the destruction of valuable compounds and develop a simple and rapid approach for obtaining drop-in hydrocarbon fuels via algae grown from flue gas. New methods are established for a direct transesterification of raw algae biomass as well as crude lipid purification. Activated carbon is utilized as a stationary phase in the purification procedure and various approaches are examined in order to optimize time and cost efficiency. Raw algae, crude lipids, purified lipids and upgraded lipids are analyzed throughout the work in order to obtain a complete profile. Complete lipid profiling and elemental analysis are performed on all algae and lipid samples as well as UV-Vis measurements and gas chromatography analysis. Thermogravimetric analysis is performed on spent materials such as the activated carbon and the catalysts used in the upgrading process. Activated carbon was found to be an effective adsorbent for the elimination of impurities such as chlorophyll, phospholipids and sterols from the crude algae oil. Comparison of the UV-Vis spectra of a chlorophyll standard, the crude algal lipids and the purified algal lipids reveals a complete absence of chlorophyll in the purified sample.

PHOTOCATALYTIC REDUCTION OF CO₂ ON α -Fe₂O₃/K₂O HETEROSTRUCTURE USING SOLAR ENERGY**Kayvon Ghayoumi, Senior, Chemistry, University of Kentucky**Ruixin Zhou, Chemistry, University of KentuckyMuthu Gnanamani, Chemistry, University of KentuckyKenneth Graham, Chemistry, University of KentuckyMarcelo Guzman, Chemistry, University of Kentucky

Photocatalytic reductions are attracting attention as a promising technology to convert CO₂ to high energy fuels using solar light. However, traditional photocatalysts suffer many limitations, including restricted light absorption ranges, poor charge separation and redox ability. This work explores the use of a novel α -Fe₂O₃/K₂O heterostructure photocatalyst to overcome many of the drawbacks of traditional photocatalysts. The α -Fe₂O₃/K₂O nanocomposite is synthesized and tested for CO₂ reduction showing an enhanced photocatalytic activity relative to its pure counterpart α -Fe₂O₃. The heterojunction formation and characterization of Type II band alignment of the composite are performed by diffuse reflectance UV-visible spectroscopy (DRUVS), ultraviolet photoelectron spectroscopy (UPS), and X-ray photoelectron spectroscopy (XPS). Upon irradiation at $\lambda \geq 295$ nm of α -Fe₂O₃/K₂O in the presence of water vapor as the hole scavenger, the photoreduction of CO₂(g) proceeds selectively to generate CO(g). The apparent quantum efficiency for CO production (Φ_{CO}) will be reported. This poster will propose a reaction mechanism based on current experimental observations. This work provides new insight to understand fundamental principles needed to photocatalytically reduce CO₂ with α -Fe₂O₃/K₂O.

MTOR SIGNALING IN BRAIN OF A UNIQUE RAT MODEL OF PARKINSON DISEASE**Sarah Goebel, Senior, Chemistry, University of Kentucky**

Parkinson's disease is the second most common age-related neurodegenerative disorder. The pathways of disease progression are not completely understood, but issues with glucose metabolism are thought to lead to a large portion of the neuronal death that occurs. Insulin is an important hormone with many functions including aiding glucose metabolism. When this process is halted, insulin resistance occurs. Previous research has shown a link between the mTOR pathway and insulin resistance in patients diagnosed with Alzheimer disease, another prevalent neurodegenerative disease. Therefore, it was proposed that activation of the PI3K/Akt/mTOR pathway could also lead to insulin resistance in a unique rat model of Parkinson's disease. This particular study involved analyzing the mTOR metabolic pathway as the disease progressed in the brain of the PINK1 KO rat, a model of inherited Parkinson disease. PINK1 is a mitochondrial kinase, mutations in which lead to inherited Parkinson disease. Three male and three female rats were analyzed from four different age groups: 2 month, 4 month, 6 month, and 8 month. The poster will present the results of our study thus far. Continued study of this system may yield important new insights into the role of mTOR signaling in Parkinson disease, with potential identification of new therapeutic targets for this devastating neurodegenerative disease.

This work was supported in part by a NIH (NINDS) grant to Dr. D. Allan Butterfield.

**COMPARISON OF SUBSTRATE BINDING TO A
HYPERTHERMOPHILIC VS. A MESOPHILIC FLAVOENZYME****Zachary Griffith, Senior, Chemistry, University of Kentucky**Anne-Frances Miller, Chemistry, University of KentuckyJohn Hoben, Chemistry, University of Kentucky

Understanding the intricacies of enzymes and their interactions with their substrates and cofactors is an integral part of many mechanistic studies, opening the possibility of manipulating the enzyme or its environment to cause desired outcomes. In this study, the focus was on a class of enzymes called flavoenzymes. Flavoenzymes make use of a flavin-based cofactor, for example flavin adenine dinucleotide (FAD) or flavin mononucleotide (FMN), to effect redox reactions central to energy metabolism and respiration. Flavin cofactors facilitate two- or one-electron redox chemistry due to their highly conjugated structure. The same electronic structure also makes flavins fluorescent and responsive to binding of pi-conjugated substrate analogues. It was hypothesized that the analogues able to donate electrons could quench flavin fluorescence by charge transfer and that this would provide insight into the cofactor's capacity for single electron acceptance. As can be expected, protein dynamics can play a major role in how substrates interact with the active site flavin upon binding. Using fluorescence emission analysis, binding with a shared substrate analogue (n-Phenylanthranilic acid) was compared for two flavoenzymes (Thermus thermophilus NADH Oxidase and Enterobacter cloacae Nitroreductase), over a range of temperatures to determine whether the two enzymes experienced different dynamics modulated by temperature, given that one enzyme derives from a hyperthermophile whereas the second derives from a mesophile.

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DEGRADATION OF DENTIN BONDING

Christopher Haas, Senior, Chemistry, University of Kentucky

Richard Mitchell, College of Dentistry, University of Kentucky

Jason DeRouchey, Chemistry, University of Kentucky

A useful tool in the world of dentistry is the utilization of adhesives to bond and seal dental filling to the tooth. While capable of producing a strong initial bonding, dental adhesives tend to degrade and break over time causing the filling to leak or the bonding to fail. The purpose of this experiment is to develop a method to measure the fracture energy to move a crack along the interface between bovine dentin and an acrylic polymer bonded to that dentin. Bonding as accomplished using an etch and rinse approach. This is where phosphoric acid removes the smear layer, dissolving the mineral component of the dentin (hydroxyapatite), leaving the collagen fibrils that can be penetrated by hydrophilic polymer "primer". Dental polymer filling materials will copolymerize with the primed dentin and therefore bond to that dentin. We will be measuring the fracture energy in order to better understand bond degradation and the effects of oral fluids on that degradation. We have used a modified double cleavage drilled compression (DCDC) test to measure fracture energy of resins bonded to dentin. The first time this fracture energy has been measured.

EFFECT OF LIGAND IDENTITY ON QUANTUM DOT SENSITIZED SOLAR CELL PERFORMANCE**Natalie Hendrix, Senior, Chemistry, Transylvania University**Kyle Schnitsenbaumer, Chemistry, Transylvania UniversityJamie Snyder, Chemistry, Transylvania University

Quantum dot sensitized solar cells have the potential to improve solar cell devices. One promising direction of research is the post synthetic modification of quantum dot surface ligands. A smaller ligand has shown to improve device performance because there is less distance between the TiO₂ paste and the quantum dot, aiding in more efficient electron flow. Cadmium Selenide quantum dots have shown to be a suitable candidate for the fabrication of the solar cells. Solar cells are constructed using FTO conductive glass, TiO₂ paste, and an electrolyte solution to help facilitate electron flow. In this project, quantum dot solar cells, utilizing surface ligands of varying lengths and chemical nature, were constructed and measured for their efficiency. The size of the quantum dot, the temperature, ambient light, and the angle of incident light were kept constant for each solar cell to identify how quantum dot ligand identity affects the performance of the device.

CARBON BASED CATALYSTS FOR CO₂ REDUCTION**Sidney Herrell, Senior, Chemistry, University of Kentucky**Namal Wanninayake, Chemistry, University of KentuckyDoo Young Kim, Chemistry, University of Kentucky

Significant buildup of greenhouse gas in the environment is a global issue due to the increasing use of fossil fuels. Therefore, the electrochemical reduction of carbon dioxide using renewable energy is important to reduce the anthropogenic CO₂, which is one of the major contributors to the greenhouse effect. The search for an efficient and durable catalyst for the electrochemical reduction of CO₂ is an active area of research because of the advancements it can lead to in the science and technology of energy conservation and environmental remediation. The electrochemical reduction of CO₂ is dependent on an effective catalyst that reduces the overpotential of the reaction, is selective toward desired products, is durable, and finally, a catalyst that suppresses the hydrogen evolution reaction which occurs during the same potential region and competes with CO₂ reduction process.¹ Development of suitable catalysts for this process, however, is challenging due to the lack of understanding of the catalytic process and limited number of efficient and robust catalysts. Recently, it has been shown that nitrogen-doped carbon shows a great promise towards electrocatalytic reduction of CO₂. N-doped carbon-based materials possess high conductivity, a low free energy barrier for the activation of the CO₂ reduction reaction, and allow suppression of the hydrogen evolution reaction.² However, the role of nitrogen species and the sp²/sp³ carbon moieties for electrocatalytic reduction of CO₂ is still ambiguous. Therefore, this research will focus specifically on the use of nitrogen doped carbon-based substrates as catalysts for CO₂ reduction and understanding the role of nitrogen species and the sp²/sp³ carbon content of the catalyst. In this project, microwave plasma enhanced chemical vapor deposition technique was used to grow N-doped carbon based catalysts with different sp²/sp³ carbon ratios. A customized electrochemical cell with a large working electrode surface area was used to enable detection of products with high sensitivity. Products from the electrochemical reaction were characterized using gas chromatography and nuclear magnetic resonance. The nature of the nitrogen-doped electrocatalysts were characterized using scanning electron microscopy, transmission electron microscopy and X-ray photoelectron spectroscopy. Results from this study indicates that the nature of the microstructure of carbon-based catalysts, paired with a better understanding of CO₂ reduction reaction kinetics, will enable the development of next generation nitrogen doped carbon based catalysts and thus improves the energy conservation techniques, and also the current state of the environment.

ELECTROLESS PLATING ON PLASTICS**Braxton McFarland, Senior, Chemistry, University of Kentucky**

Electroless copper plating is a process similar to plating from a galvanic cell, but does not require an external energy source. The auto catalytic reaction occurs in a plating bath and results in a metal layer plated on top of a substrate. A plating bath is comprised of a reducing agent, complexant, stabilizer and ion source. The electroless method often involves plating metal onto other metal substrates, but also has the capability of plating metal layers on to plastics. We have determined an effective electroless plating process using nonmagnetic materials suitable for an electromagnetic coil as a 3-d printed circuit.

AB9 ESTERS – SYNTHESIS AND CHARACTERIZATION**Ryan Melody, Senior, Chemistry, University of Kentucky**David Atwood, Chemistry, University of Kentucky

Bidentate dithiol 2,2'-(isophthaloylbis(azanaediyl)bis(3-mercaptopropanioc acid)) (Trade names: ABDTH2 or AB9) is a chelating agent of interest due to its high affinity for heavy metal ions in solution and compatibility with silica attachments. Characterization of magnetic nanoparticle coupling and physical properties has been documented, but due to the complete insolubility of AB9, crystallization has proven unsuccessful.

The purpose of this research project is to synthesize the methyl (ME-AB9) and ethyl (EE-AB9) esters of AB9 and characterize both the complexed and un-complexed structures associated with each ester. Characterization will be performed through techniques such as Infrared Spectrometry, H1-NMR, TGA, DSC, and various crystallization techniques such as vapor diffusion, slow evaporation, and slow cooling. This characterization data has provided fundamental information about the structure and bonding of AB9 and AB9 analogs.

EFFECTS OF THE WATER CONTENT IN LEAD ACETATE ON MORPHOLOGY AND PV PERFORMANCE OF METHYLAMMONIUM LEAD HALIDE PEROVSKITES

Thuy Nguyen, Senior, Chemistry, University of Kentucky

Kenneth Graham, Chemistry, University of Kentucky

So Min Park, Chemistry, University of Kentucky

Inorganic perovskites have made a breakthrough in solar cells for lower cost and high performance compared to the mass produced silicon solar cells. Due to the difficulties during the fabrication process, reproducibility in these type of cells is relatively poor. Specifically, planar heterojunction methylammonium lead iodide (MAPb3I) perovskite solar cells are highly sensitive to air, annealing time, solvent, and various methods of fabrication. Which lead to the investigation of the effects from purity, brand, and water content of the lead acetate trihydrate, Pb(Ac)₂ precursor on the performance of the PV cells. Although, the lead acetate photoluminescence properties and external quantum efficiency in the sub-bandgap region increase with increasing purity; its performance is often lowered due to other factors. While determining the appropriate amount of water content in the lead acetate had a significantly positive effect on the PV performance and morphology of the films compared to the commercially bought and the dehydrated forms. Optimization of the effects of lead acetate has the potential for as a controllable, reproducible precursor for MAPb3I perovskite solar cells.

LAND USE HISTORY, SOIL CHARACTERIZATION AND INVASIVE SPECIES IN THE BEREA COLLEGE FOREST.**Savannah Osborne, Senior, Chemistry, Berea College**

Berea College manages about 9000 acres of forest land that is a valuable part of student life and learning at the college, and is listed on the National Register of Historic Places. The first College Forester was Silas C. Mason (1897-1908), who began land acquisition with his own funds. Most of the newly purchased land was abandoned logged-over land, pasture or cropland. Closely associated today with historical land clearance is the dominance in the understory of invasive exotic woody species, including Japanese honeysuckle (*Lonicera japonica*) and bush honeysuckle (*Lonicera maackii*) among others. To combat the spread of the invasives, the Forestry Unit uses glyphosate herbicide (Rodeo™ brand). We sampled 5 sites comprising 4 soil series in two areas of the College Forest where invasive species are a problem, and characterized the soils chemically and physically. Surface soils at most sites were very strongly acid (pH in water 3.8 to 4.4) with surface texture of clay loam to silt loam, and organic matter 3 to 44%. Two sites at the northern and southern ends of the 60-acre treatment area on the cross-country trail section of the forest (Blago and Captina soil series) were chosen for further study.

CHARACTERIZATION OF RECOMBINANT ENL-YEATS DOMAIN AND IT'S PROTEIN-PROTEIN INTERACTION WITH Paf1**Egan Peltan, Senior, Biochemistry, Transylvania University**Sierrah Grigsby, Pathology, University of MichiganZaneta Nikolovska-Coleska, Pathology, University of Michigan

The YEATS domain is a highly-conserved sequence motif present in a diverse family of chromatin associated proteins. Previous studies have demonstrated that YEATS domain family proteins exhibit acetyllysine (H3Kac) and crotonyllysine (H3Kcr) binding activity.^{2,3} Furthermore, two YEATS proteins, AF9 and ENL, have also been reported to interact with PAFc through its Paf1 subunit as part of the Super Elongation Complex (SEC).⁴ To characterize this interaction, recombinant ENL-YEATS (ENL 5-140) was constructed, expressed, and purified to confirm its non-histone binding activity with Paf1 via Biolayer Interferometry.

IMPROVED MICROWAVE DIGESTION METHODS FOR BONE ASH AND PORTLAND CEMENT**Amy Rice, Senior, Chemistry, Thomas More College**Kelsey Kaht, Chemistry, University of LouisvilleWilliam Wetzel, Chemistry, Thomas More CollegeChrista Currie, Chemistry, Mount Saint Joseph University

In the early 2000s, a crematorium in Georgia unethically disposed of deceased bodies and provided families with cement in place of authentic cremated remains. Since that time, a variety of methods have been explored to differentiate human cremated remains from other materials. Previous work in our lab has been directed at using two certified reference materials, Bone Ash (NIST 1400) and Portland Cement (NIST 634a), as a model for human cremated remains and other (non-cremated remains) materials. Bone Ash or Portland Cement were dissolved in nitric acid and hydrogen peroxide using microwave-assisted digestion and the resulting solutions were analyzed using Inductively Coupled Plasma-Atomic Emission Spectrometry (ICP-AES). In this work, alternative digestion vessels capable of withstanding higher temperatures and pressures were evaluated for the digestion of bone ash and cement. Preliminary results suggest that the high-temperature/high-pressure reaction vessels offer a more complete digestion of the standard reference materials and a corresponding improvement in the accuracy of precision of the results.

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DEFINING ABDTH2 (AB9)

Britteny Ruggles, Senior, Chemistry, University of Kentucky

Water remediation is an imperative aspect of maintaining clean water sources. An active area of research is developing compounds to remove heavy metals from high-risk water sources. This project focuses on synthesizing ABDTH2 (AB9), a compound capable of binding heavy metals and main group elements that form stable insoluble precipitates. The goal is to characterize un-complexed AB9 and complexed AB9 with various heavy metal ions. Characterization will be met through determination of solubility constants with a variety of common solvents, melting point, IR, quantifying ion capture of metal contaminants in solution, and developing a crystalline structure of AB9.

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IRON-CATALYZED SUBSTITUTION OF ALCOHOLS

Julie Simon, Sophomore, Chemistry, Indiana University

Paul Marcyk, Chemistry, Indiana University

Silas Cook, Chemistry, Indiana University

Alcohols are attractive electrophiles for alkylation as they are widely available, stable and easy to prepare. The Cook group has developed a novel catalytic system to activate alcohols for substitution with nitrogen and arene nucleophiles. My research involves using this system for the activation of alcohols substitution reactions with oxygen and sulfur. Intramolecular substitution with oxygen was successful, but the product underwent undesired Friedel-Crafts Alkylation. Future work will involve adding electron-withdrawing groups in order to deactivate the product from this side reaction. Intramolecular substitution with sulfur has not yet been attempted. Future work will involve identifying a suitable protecting group to synthesize the starting material and attempting the intramolecular substitution.

DIFFERENCES IN THE MEMBRANE EXPRESSION OF GPR39 IN THE PRESENCE AND ABSENCE OF ZINC IONS**Kimberly Stevens, Senior, Chemistry, University of Kentucky**Mark Lovell, Chemistry and Sanders-Brown Center on Aging, University of KentuckyChris Richards, Chemistry, University of Kentucky

GPR39 is a member of the G-protein-coupled receptor family and is expressed throughout the body including the central nervous system as well as the digestion track. This protein has been found to play a role in numerous physiological processes such as the secretion of insulin, digestion, and wound healing. It has also been implicated as playing a role in obesity and depression. New studies suggest it may even contribute to Alzheimer's disease. Although it is still considered an orphan receptor, GPR39 appears to be primarily activated by Zn^{2+} ions and thus has a unique role as a membrane protein in Zn^{2+} sensing. The purpose of this research was to study the expression of GPR39 on the cell membrane and to compare this to the membrane expression of the protein in the presence of Zn^{2+} ions. To do this, the protein was first tagged with the fluorescent protein Super Ecliptic Phluorin (SEP) in order to visualize the protein in live cells. HEK cells were cultured and transfected with the construct and imaged using Total Internal Reflection Florescence (TIRF) Microscopy with a 488 nm wavelength laser. This technique implements the fundamental laws of reflection to excite only fluorophores near the cell surface allowing for membrane expression and insertion events into the membrane to be studied.

PREDICTION OF HYDROXYLATION RATE CONSTANTS FROM MOLECULAR STRUCTURE BY CHEMINFORMATICS METHODS WITH COMPUTATIONAL NEURAL NETWORK

Darin Vaughan, Junior, Chemistry and Mathematics, Morehead State

Pharmaceutical drug discovery and design has always been a complicated and time consuming process, especially for purely experimental chemists. This study presents a highly interdisciplinary approach to solving difficult problems in drug discovery through cheminformatics.

Quantitative structure-activity relationship models are a multiple linear regression technique for aiding in predicting certain properties of compounds, such as the relationship between the chemical structure of an enzyme inhibitor and its biological activity. To explore the strength and utility of QSAR methods, a model was developed relating three classes of structure descriptors for a set of unsaturated hydrocarbons which undergo hydroxylation reactions to accurately predict k_{OH} rate constants. To aid in the advancement of novel and promising technology, computational neural networks (commonly named Artificial Neural Networks) were employed for producing a predictive learning model which resulted in exceptionally low error.

This technique provides a strong measure of confidence for scalability into more complex molecular relationships such enzyme reaction rates which are important for Michaelis-Menten dynamics. The time saving benefit of QSAR and cheminformatics in general is that enzyme assays and extensive reaction spectroscopy are not necessary to determine rate constants. Reaction dynamics may be simulated entirely in silico using such a multidisciplinary approach as this. Combining relatively accessible methods from computer and data science, quantum computational chemistry, applied mathematics, and organic and pharmaceutical chemistry, cheminformatics provides the opportunity for people from any discipline to enter an exciting field.

TETRAZOLE SYNTHESIS THROUGH CLICK CHEMISTRY REACTION**Jacob Walker, Junior, Chemistry, University of Kentucky**Dr. Daniel Esterline, Chemistry, Thomas More College

“Click Chemistry”, a newly discovered set of rules founded by Dr. Barry Sharpless, was first introduced at the 217th American Chemical Society’s annual meeting. Differing from most other theories in organic chemistry, “Click Chemistry” is not limited to a single type of reaction, but rather govern how many different reactions can be performed, using specific, “easily made” reactants to mimic the reactions that have occurred in nature. Specifically, the synthesis of a specific tetrazole, 2-benzyl-5-phenyl-2H-tetrazole, was attempted using the common Click Chemistry reactant, benzyl azide. Benzyl azide must first be synthesized prior to the tetrazole synthesis. The synthesis of benzyl azide was performed a few times on a large scale to ensure an adequate amount of reactant was accessible to perform the Click Chemistry, reaction between benzyl azide and various nitriles. The product of the Click Chemistry reaction was then analyzed using multiple spectroscopic methods to determine if the reaction was successful or not.