

ABSTRACTS

Department of Chemistry
Regional Undergraduate
Poster Competition
Jacobs Science Building
April 15, 2022
11:30am - 3:30pm

Department of Chemistry
University of Kentucky
Lexington, KY 40506

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*Group A presents from 12:00pm to 1:30pm.

*Group B presents from 1:30pm to 3:00pm.

1

USING ELISA ASSAYS TO UNDERSTAND HOW INSULIN-DEGRADING ENZYME GAINS ACCESS TO ITS SUBSTRATES

Darcy Adreon, Junior, Chemistry, University of Kentucky

David Rodgers, Molecular & Cellular Biochemistry, University of Kentucky

Abstract:

Insulin-degrading enzyme (IDE) is a peptidase that metabolizes signaling and other peptides including insulin and amyloid- β , making it a promising target for therapeutics. Of special interest is the mechanism by which IDE, an enzyme produced in the cytosol, encounters its substrates, which are typically taken up into endosomal compartments within the cell. It is hypothesized that IDE encounters its substrates by first localizing to endosomes through interactions with phosphatidylinositol phosphate (PIP) lipids contained within the membrane. The proposed mechanism of localization is via PIP head group interaction with a site near the surface of the enzyme located at the interface between the two halves of IDE, which has a clamshell-like overall architecture. Previous docking studies with portions of the PIP head group identified this site.

Research aims to test the proposed PIP interaction site and secondarily to determine affinity differences for different PIP lipids found in various cellular membranes. The interaction site is being tested by determining the effect of mutations in the site on binding to artificial membranes known as liposomes, which contain PIP lipids. Finding that mutations in the site decrease or abrogate binding to PIP-doped liposomes would provide strong support for it mediating the interaction with PIP lipid head groups. The binding of IDE to liposomes is measured using a sandwich enzyme-linked immunosorbent assay (ELISA), which allows the binding affinity to be determined in the form of a dissociation constant. Experimental results support the proposed binding site, with two variants, IDE^{Q129E,R824A,R892A,H885A} and IDE^{Q129E,N821A,Y831A,H885A}, showing almost no interaction with phosphatidylinositol 4,5-bisphosphate-doped liposomes. Early results with different PIP lipids show relatively minor affinity differences. In future work, IDE variants that lack PIP binding will be used to test the proposed mechanism of localization to endosomal compartments in cultured cells.

2

MEASURING THE TEMPERATURE-DEPENDENT FLUORESCENCE OF RHODAMINE DYES AND INP-BASED QUANTUM DOTS

Saif Ahmed, Junior, Chemistry, Transylvania University

Alyssa Nguyen, Transylvania University

Kyle Schnitzenbaum, Chemistry, Tansylvania University

Abstract:

The emission intensity of a fluorophore is closely linked to the temperature of its surroundings. The objective of this project was to measure the fluorescence of several dyes and quantum dots across a wide range of temperatures. Attention was primarily paid to the Rhodamine family of dyes (specifically Rhodamine B, 6G, and 101) and quantum dots that contained an InP core with either a ZnSe or ZnS shell. The dyes were dissolved in an ethylene glycol solvent while the quantum dots were suspended in octadecene. The absorption, fluorescence excitation, and fluorescence emission of these fluorophores were measured at regular intervals from 20° C to 140° C and then back down to 20°C. The results of this project demonstrate that the Rhodamine dyes exhibit thermal quenching to varying degrees depending on molecular structure. For all three dyes the quenching was found to be reversible upon cooling. This contrasts with the quantum dots, whose fluorescence intensity was permanently quenched due to an increase in temperature.

3

OPTIMIZATION OF THE FERROZINE ASSAY TO DETERMINE FREE IRON IN SOLUTION

Mary Asante, Senior, Chemistry, Ball State University

Mary Konkle, Chemistry, Ball State University

Abstract:

The accumulation of free iron in biological systems can be very dangerous due to the Fenton chemistry that it catalyzes and then produces reactive oxygen species. Previous research showed that the diabetes drug target mitoNEET has a labile [2Fe-2S] cluster. The stability of the cluster of mitoNEET can be influenced by ligands, ligating residues, and the pH of the environment. Prior results from the Konkle laboratory showed that mitoNEET is reactive towards the cellular electrophiles 4-hydroxynonenal and 4-oxononenal which are produced from Fenton chemistry. The ferrozine assay is a spectrophotometric method of determining free iron ions in solution. In this work, the ferrozine assay was optimized to determine the cluster loss from mitoNEET. Additionally, addition of HNE and ONE were assayed to determine the impact of their modification of mitoNEET on its cluster stability. If modification of mitoNEET by HNE or ONE causes further release of iron, then a cycle of perpetuating oxidative stress would be established.

4

SURFACE ENERGY PROFILING OF ADHESIN PROTEINS

Pedro Henrique Ayres Galhardo, Senior, Chemistry & Biochemistry
Lipscomb University

Alexus Brown, Chemistry & Biochemistry, Lipscomb University

Abstract:

Common infections caused by microorganisms, such as urinary tract infections and blood infections, are often exacerbated by the formation of bacterial biofilm. Biofilms greatly increase the survivability, resistance, proliferation, and infectious character of harmful bacteria such as *Escherichia coli* (E.coli). Studies have shown that biofilm formation occurs in five stages and that the initial step, primary colonization, is the only form of reversible attachment, thus making it a prime candidate for intervention. As such, the purpose of this research is to better understand the thermodynamic nature of said reversible binding. This will be done by determining the Gibbs energy of attachment of E.coli adhesion proteins, FimH and PapG, and other pili proteins that play pivotal roles in the binding process, such as FimA and PapF. The Gibbs energy represents the spontaneity of the attachment process and through this determination, it is possible to formulate a surface energy postulate that predicts the interaction of different microorganism and substrate combinations. The determination method is simple and relatively inexpensive as it employs goniometric techniques. Ultimately, this research would allow for the design of affordable materials that are biofilm resistant, and lead to the reduction of pathogen proliferation.

5

IMPACT OF ANION EXCHANGE ON ORGANIC SEMICONDUCTING POLYMER FILMS

Ahmed Ayyash, Senior, Chemistry, University of Kentucky
Kenneth Graham, Chemistry, University of Kentucky

Abstract:

There has been a recent surge in the interest of organic semiconducting polymers (OSP) for their use in sensing, bioelectronics, flexible electronics, and organic electrochemical transistors. It is important to improve the doping processes of OSPs since this will allow for further understanding of how to effectively apply these materials in the before mentioned settings. OSPs possess a unique characteristic where their electrical properties can be tuned based on the counterions that are included in the doped films. An emerging technique of doping OSPs involves the method of ion exchange doping (IED). The process of IED involves the use of an initial dopant ion that is then exchanged with different counter anion, this process occurs spontaneously by adding a large excess of an electrolyte solution that contains the desired counter ion. If this process is performed efficiently, then only the electrolyte counter ion should remain in the film. This research project will focus on the ion exchange efficiency of various polymers by initially doping the polymer films with FeCl₃ then exchanging the Cl⁻ ions with the following counter ions: bis (trifluoromethanesulfonyl)imide (TFSI⁻), Tetrafluoroborate (BF₄⁻), 3,5-bis(trifluoromethyl)phenyl borate (BARF). The effect of the counter ions on the polymer films was determined by testing the Seebeck coefficients, sheet resistance, and UV-Vis absorbance of the films. From this study it was found that the films reach their doping capacity within 30 – 60 seconds of exposure to the dopant solution which was confirmed by the similar Seebeck coefficients and Sheet resistance measurements of the films that were exposed for 30 and 300 seconds. All of the films have shown similar Seebeck coefficients and sheet resistance values regardless of the time of exposure.

7

CHARACTERIZATION OF PROTEIN NECESSARY FOR THE SURVIVAL OF *A. BAUMANNII* IN LOW-ZN CONDITIONS

Christopher Basile, Senior, Chemistry, Indiana University

Sambuddha Sen, Chemistry, Indiana University

David Giedroc, Chemistry, Indiana University

Abstract:

Transition metal ions are important cofactors in countless proteins necessary for cellular function. Because of this importance, transition metals such as zinc are frequently sequestered by hosts in response to bacterial infections in a process termed nutritional immunity. Study of *Acinetobacter baumannii*, a common hospital-acquired antibiotic-resistant pathogen, under conditions of Zn starvation revealed the gene A1S_0780 was absolutely necessary for survival. This gene encodes a homolog of the eukaryotic protein Cfd1, which is involved in the maturation of proteins with Fe/S clusters. This study sought to characterize this bacterial Cfd1 and elucidate its role in the response to Zn starvation. Cfd1 was unable to compete with the indicator Mag-Fura-2, suggesting the protein does not directly bind Zn ions. The protein was found to have both ATPase activity and the ability to transfer Fe/S clusters to other proteins, suggesting it has similar function to the eukaryotic protein. Site-directed mutagenesis was used to develop mutants of Cfd1. A lysine residue in a deviant Walker A motif was found to play an important role in its ATPase activity, and a mutation of two cysteine residues in a CXXC motif was found to eliminate the ability to bind Fe/S clusters. It is thought that the protein assists in the development of another protein that is impacted by Zn starvation. Future studies will probe the interaction between Cfd1 and the NuoF subunit of respiratory complex I, which possesses both Fe/S clusters and flavins which may be impacted by a low Zn environment. Cfd1's importance to the survival of *A. baumannii* suggests it may be an important target for treatment.

8

SYNTHESIS OF HYBRID ORGANIC-INORGANIC COMPOUNDS FOR POTENTIAL USE IN ORGANIC LIGHT-EMITTING DIODES (OLEDs)

Eric Bias, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

Abstract:

Organic light-emitting diodes (OLED) are growing increasingly present in our technological devices from the cellphones in our pockets to television screens in our homes. One of the key components of an OLED is the charge transport materials, which facilitates the transfer of charges from the device's metal electrodes to or from the light-emitting material. Current device efficiencies are hampered by the low charge conductivity of state-of-the-art charge transport materials. Therefore, this project is primarily concerned with making novel materials that can transport charges more efficiently. Our approach to synthesizing these materials is to utilize hybrid organic-inorganic materials, which have an organic cation and an inorganic anion that crystallize in a controlled manner. The plan for this project is to 1. synthesize several different organic cations and 2. combine them with different inorganic anions and then 3. measure how well the materials conduct electric charges. Progress towards these three goals will be discussed in this poster.

9

INKJET PRINTING AG ELECTRODES TOWARDS ELECTROCHEMICAL SENSORS

Kelsey Blackford, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

Abstract:

Printed circuits prove to be important and extremely beneficial to the world today. They are desirable due to their potential cost effectiveness and compatibility with flexible substrates. The initial aim of this research was to create an affordable, yet reliable sensor for selective drug detection. It was important that this sensor was able to maintain its accuracy with a relatively small amount of sample present, and so an inkjet printing strategy was chosen, since inkjet printing can reproducibly produce high resolution patterns. A small molecule silver precursor-based ink was synthesized, and rheological data (density, viscosity, and surface tension) measured. Polyester (PET) proved to be the best substrate for the ink to be printed onto after initial printing trials on paper, glass, and PET. Through intense UV flash photo curing, the dried, resistive Ag films were converted to conductive films (<2 Ohms resistance). A three-electrode pattern was designed and reproducibly printed on PET, to be used as working electrode, counter electrode, and reference electrode. A potentiostat was used to test durability of the electrodes in solution over time. Multiple layers of ink followed by photocuring proved to create the most durable electrode over time.

**SYNTHESIS AND CHARACTERIZATION OF STABLE GOLD (III)
DITHIOCARBAMATE COMPLEXES**

James Dawahare, Junior, Chemistry, University of Kentucky

Samuel Awuah, Chemistry, University of Kentucky

Adedamola Arojoye, Chemistry, University of Kentucky

Abstract:

Mitochondrial respiration is a viable therapeutic target that is relatively unexplored in anti-cancer drug discovery and development. Recent studies into the mode of action of organogold (III) complexes have pointed to selective disruption of mitochondria in cancer cells. Here, we detail the synthesis, characterization, and biological activity of two neutral [C[^]C]-cyclometalated gold (III) complexes bearing dithiocarbamate ligands. Cell viability studies of the two complexes show moderate potency (about 100 μM) within the cancer cell lines (BT-333, H460, MDA-MB-231 and MDA-MB-468) studied. This work demonstrates a unique scaffold for a new generation of neutral gold(III) complexes with applications in drug discovery, catalysis, and organic electronics. Further studies into the stability, redox potential, expanded structure-activity relationship studies (SAR), mechanism of action, and functional studies in cancer cells are planned.

CHARACTERIZATION OF THERMOGELS FOR MITOCHONDRIA DELIVERY

Zoe Gallegos, Junior, Chemistry, University of Kentucky

Jason DeRouchey, Chemistry, University of Kentucky

Thomas Dziubla, Chemical Engineering, University of Kentucky

Ammar Jamie Amhed, Chemical Engineering, University of Kentucky

Abstract:

Following a spinal cord injury, a secondary series of biochemical events occur, enhancing the damage following the initial injury. Though there are numerous processes that lead to this secondary injury cascade, mitochondrial function plays a major initiating role in many of these processes. There has been promising data showing that transplanting healthy, viable mitochondria into the injury site can improve cellular bioenergetics, and therefore, prevent this secondary damage from occurring; however, the challenge arises in being able to actually deliver the mitochondria. This research focuses on characterizing an erodible thermogel system that delivers mitochondria to evaluate the phase behavior and assess level of control over the gel. The optical density evidence showed that methylcellulose (MC) is the driving factor in the phase transition, with pure MC progressively precipitating at lower temperatures as its concentration increased. Though temperature had no effect on the optical density of hyaluronic acid (HA), studies with mixed concentrations of HA and MC showed that as HA concentration increased, the precipitation temperature decreased, thus emphasizing HAMC's ability to provide a valuable mitochondrial delivery system.

CHEMICAL RECYCLING OF POLYETHYLENE TEREPHTHALATE (PET) VIA MICROWAVE-ASSISTED DEPOLYMERIZATION

Samuel Golden, Senior, Chemistry, University of the Cumberland

Sean Kennedy, Chemistry, University of the Cumberland

Julie Tan, Chemistry, University of the Cumberland

Abstract:

Plastic waste pollution has become a major environmental challenge. Around 300 million tons of plastic waste are generated globally each year, and polyethylene terephthalate (PET) is among the most used plastic in modern society. Chemical recycling of plastics to its original feedstock is a useful strategy in dealing with plastic pollution in the environment. In this context, we herein describe a facile and efficient method for depolymerizing PET into terephthalic acid (TPA). Using PET single-use soft drink bottle waste, the depolymerization was performed via base hydrolysis under microwave irradiation using a domestic microwave oven. The depolymerized product, TPA, was obtained in sufficiently high yield. This result illustrates the importance of the microwave-assisted technique as a promising recycling method for plastic bottles made from PET, which resulted in TPA feedstock recovery. This method of depolymerization of PET can be accomplished in a typical lab period in the undergraduate organic chemistry laboratory and it is particularly fitting when it is related to the ester hydrolysis topic in the organic lecture.

CU₂O/BIOBR HETEROSTRUCTURES FOR PHOTOCATALYTIC DEGRADATION OF EMERGING ORGANIC CONTAMINANTS

Albert Gonzalez, Sophomore. Chemistry, Ball State University

Elsayed Zahran, Chemistry, Ball State University

Abelline Fionah, Chemistry, University of Kentucky

Abstract:

Emerging organic contaminants have recently been recognized as a threat to human health and the ecosystem. In this poster, we introduce a method to prepare controlled heterostructures of Cu₂O/BiOBr via a low-temperature hydrothermal procedure. The size, composition, morphology, and structure of the material were characterized by electron microscopy, energy dispersive spectroscopy, x-ray diffraction, x-ray photoelectron spectroscopy, BET surface area, and diffuse reflectance spectroscopy. The activity of the Cu₂O/BiOBr photocatalyst was evaluated in the degradation of rhodamine B and methyl orange organic dyes. Tuning the composition of the heterostructures led to significant improvement in the photocatalytic degradation of both cationic and anionic organic contaminants. The photocatalyst demonstrated substantial activity in the degradation of methyl orange by a combined effect of adsorption in dark and photocatalysis. The mechanism of the methyl orange degradation was investigated in dark and under light irradiation by using radical scavengers. The multicomponent Cu₂O/BiOBr photocatalyst demonstrated rapid mineralization of glyphosate, a widely used herbicide that has shown adverse effects on human health.

**EFFECT OF ENVIRONMENT ON ANION-PI INTERACTIONS
BETWEEN PARA-SUBSTITUTED BENZOQUINONE PI-ACCEPTORS
AND HALIDE ANIONS**

Devin Howe, Senior, Chemistry, Ball State University

Josh Wilson, Chemistry, Ball State University

Sergiy Rosokha, Chemistry, Ball State University

Abstract:

The formation of anion- π bonding complexes between para-substituted benzoquinone π -acceptors and halide anions had been observed quantitatively and evaluated qualitatively using UV-Vis spectroscopy. This allowed us to analyze how solvent polarities and the presence of ionic salts (varied ionic environment) affect complex formation. From the absorption data collected from UV-Vis spectroscopy, computational methods were applied to calculate formation constants, K . For low ionic strength, K was larger for complex formation in dichloromethane solvent than in the more polar acetonitrile solvent. Interaction energies (ΔE) obtained by quantum mechanical computations were also decreased with the more polar solvents. For high ionic strength, K was smaller for complex formation in dichloromethane when compared to acetonitrile. These were assigned to competing complex formation between π -acceptors and anions from the supporting electrolytes added to adjust ionic strength. This study shows that solvent polarity and ionic environments should be considered for analysis of the strength of anion- π interactions and its applications.

IDENTIFYING MAJOR SURFACE ATTACHMENT PROTEINS THAT AFFECT EX VIVO STAPHYLOCOCCAL BIOFILM FORMATION

Leah Jacob, Freshman, Chemistry, Lipscomb University

Leah Jacob, Biochemistry, Lipscomb University

Shivani Patel, Biology, Lipscomb University

Abstract:

Present in epidermal tissues and parts of the upper respiratory tract, *Staphylococcus epidermidis* and *Staphylococcus aureus* are commonly found gram-positive bacteria in the human microbiota and are one of the leading causes of infection in the medical setting. From our research, we were able to identify a *cna* protein and two major families of surface attachment proteins: Sdr and AtI. Abiotic adhesin proteins, such as AtI proteins, are most applicable to this study. Through thermodynamic and kinetic analyses, characterization of AtI proteins' attachment mechanisms can enable us to design specific surfaces to decrease primary colonization and the resulting biofilm formation of said bacteria, thereby disrupting their infectious nature. The abiotic adhesin proteins are experimentally characterized in order to calculate relevant Gibbs energies which can be used to customize the surface chemistry of the abiotic surface to induce a non-spontaneous interaction and deter the bacteria from establishing biofilms on the surface. In this poster, we will present a study of the proteins that will be most meaningful for inhibiting Staphylococcal biofilm formation on abiotic, ex vivo surfaces.

YEAST FERMENTATION OF EXOGENOUS FATTY ACIDS FOR ESTER PRODUCTION ANALYZED BY GC-MS

Kyle Kmiec, Senior, Chemistry, University of Kentucky

Bert Lynn, Chemistry, University of Kentucky

Abstract:

Esters are an important source of flavor in distilled spirits. Unfortunately, there are many myths and legends about the origins of esters in spirit production. In this work, we attempt to shed some light on yeast derived esters and how these esters can be tuned for a particular flavor expression. With the addition of unnatural fatty acids (such as undecanoic acid) into a fermentation cycle, the propagation of fatty acid esters can be altered. Using GC-MS, we determined the normal distribution of fatty acid esters of a standard fermentation and compared this data to the experimental fermentations. Through this comparison we can see that adding in an excess amount of undecanoic acid leads to ethyl undecanoate dominated yeast ester production, and the yeast failed to produce the normal spread of fatty acid esters in a fermentation. By adding in a small amount of the undecanoic acid instead of an excess amount, the ethyl undecanoate can be seen but much less prominent along with other natural esters. Therefore, if a fatty acid is added into the fermentation, the yeast will use up that fatty acid first before producing other natural fatty acid esters that are commonly seen in a distilled spirit.

**CREATION OF CIS AND TRANS ISOMERS FOR 1,3-DIPOLAR
CYCLOADDITION AND THE PRODUCTION OF STEREOSPECIFIC
DIAMINES**

Amanda Medina, Junior, Chemistry, University of Kentucky

Robert Grossman, Chemistry, University of Kentucky

Abstract:

The goal of this project is to see whether cis and trans isomers retain stereochemistry after 1,3-dipolar cycloaddition of the alkene and azide, and then subsequent alkylation and reduction using Raney nickel to the diamine. The starting molecule used was diethyl malonate for both the cis and trans isomers. Deprotonation and addition of an alkyne was done for the cis isomer. The trans isomer was subjected to crotyl chloride and the alkene was added. The cis isomer pathway had the alkyne reduced to the alkene via the Lindlar catalyst to ensure that the cis isomer was created. Both isomers were subjected to deprotonation and alkylation with 1,2-dibromoethane. After alkylation, both isomers were then subjected to azide, which replaced the bromine. Cycloaddition was attempted on the trans isomer in methanol, acetone, and toluene, with little to no formation of the desired product and a lot of decomposition.

George Mendoza, Junior, Chemistry, University of Kentucky

Mary Konkle, Chemistry, Ball State University

Abstract:

MitoNEET is a [2Fe-2S]-cluster containing protein that is a drug target for type-2 diabetes, but the biological function of MitoNEET remains unclear. MitoNEET is a homodimer, and each monomer contains one cluster ligated by 3 cysteine (Cys 72,74, and 83) and 1 histidine (His87) residues. His87 is in a hydrogen bonding network with Lys55 of the other monomer. This creates a small 3-dimensional space lined with reactive residues. Our hypothesis is that this area is an enzyme active site and that MitoNEET functions as an enzymatic transaminase. Using spectroscopy and proteomic analysis, we determined that the coenzyme necessary for transamination, pyridoxal phosphate (PLP), binds selectively to Lys55 to form the internal aldimine. To accomplish a transamination, the two substrates need to be an amino acid (cysteine) and an α -ketoacid (pyruvate, α -ketoglutarate, and oxaloacetate). Upon addition of cysteine, the absorbance at $\lambda = 410$ nm decrease and the absorbance at $\lambda = 330$ nm increased, with an isosbestic point of $\lambda = 350$ nm. This indicated the formation of the external aldimine. When the α -ketoacid pyruvate and α -ketoglutarate were added in the presence of cysteine, the $\lambda = 330$ nm failed to increase over time. This lack of an emerging $\lambda = 330$ nm signal indicates that pyruvate and α -ketoglutarate complete the ping-pong catalytic cycle. The same was not true for oxaloacetate. The hypothetical products of this transamination done by MitoNEET are 2-mercaptopyruvate and either alanine or glutamate, depending on the α -ketoacid used. These results open a whole new area of enzymology and drug development for molecules that target MitoNEET.

EFFECTS OF LYSOSOMAL RUPTURE ON PLATELET FUNCTION**Linda Omali, Junior, Chemistry, University of Kentucky**

Sidney Whiteheart, Molecular & Cellular Biochemistry, University of Kentucky

Abstract:

Platelets are critical cell fragments most known for their role in clot formation to stop bleeding. However, they do just more than that. Platelets can endocytose - or uptake - various substances including viruses, bacterial fragments, polystyrene beads, and even soot from diesel exhaust. This then has the chance to activate said platelets. Platelets have a series of organelles in the endocytic pathway (endosomal-lysosomal system) where various cargo molecules are internalized, recycled, and modulated. Through this system, materials can be trafficked to acidic environments where they can then be degraded by hydrolytic enzymes. Pathogens may be able to manipulate this system causing lysosomal membrane permeabilization (LMP) which then triggers the rupturing of the plasma membrane and necrotic cell death. This process is known as lysosomal cell death (LCD) and causes the host cell to die. To understand whether LMP can occur in platelets and thus affect their function, we tested the effects of L-leucyl-L-leucine methyl ester (LLOMe), an acid-dependent polymer/pore forming compound that is a pH-dependent toxin, to determine if it would damage platelets and/or induce either activation by releasing calcium from the lysosome. Increasing concentrations of LLOMe led to a dose-dependent aggregation of wash mouse platelets, indicating that the pore-forming drug can cause platelet activation. Further research would need to be conducted to figure out the mechanism of the activation (i.e., ATP secretion) as well as the reagent limitations to platelet activation. In doing so, we hope to further understand various human diseases including cancer and pathogen-induced thrombocytopenia that may be caused due to LCD.

USING EXTENDED DLVO THEORY TO CHARACTERIZE PRIMARY COLONIZATION OF BACTERIA

Niyati Pathak, Senior, Chemistry, University of Kentucky
Cavitt Brian, Chemistry/Biochemistry, Lipscomb University

Abstract:

Bacterial attachment is the first step in microbe-surface interaction. Interfacial interactions exert both attractive and repulsive forces which promote growth and/or pathogenesis. The bacterial attachment could be determined by variant factors including bacterial sensing and surface chemistry. We attempt to explain bacterial attachment based on extended DLVO thermodynamic approach where the extent of bacterial adhesion to an external substrate is determined by the surface energies of the bacterium's adhesive components, substrate, and liquid medium. Interfacial interactions of the bacterial surface determined from the surface energies using DLVO theory may allow explicit prediction of the extent of bacterial attachment to different substrates. The adhesive forces may be calculated between a substrate and an interacting rod-shaped, motile bacterium or spherical, non-motile bacterium. Using the adhesive forces of the aforementioned bacteria, the individual Hamaker constants could be determined providing a quantitative description of each bacterium's mode of adhesion. The constant itself determines the macroscopic interactions through the integration of all the intermolecular interactions present between the bacterium, substrate, and liquid medium. The surface thermodynamics using extended DLVO approach could help identify the repulsive and attractive forces needed for persistent bacterial attachment to surfaces and may identify materials that would resist bacterial attachment reducing costs for industrial and biomedical applications.

USING LINEAR FUSED AROMATIC COMPOUNDS TO EXPLORE THE SYNTHESIS OF BRANCHED ALKYNE THIOL SUBSTITUENT PROCEDURES

Carleigh Phelon, Junior, Chemistry, University of Kentucky

John Anthony, Chemistry, University of Kentucky

Abstract:

The crystal engineering of linear fused aromatic compound was explored through the synthesis of highly branched alkyne substituents. This started with the reaction of 2-aminoanthraquinone and KI to produce 2-iodo-anthraquinone. Then a reaction of 4-t-butyl phenyl acetylene and the previously made 2-iodo anthraquinone. Once the product from this reaction was purified the iodine group needed to be replaced with a thiol group. On a small scale, two separate procedures were carried out to see which one resulted in the best product. One procedure called for 1,2-ethanedithiol and the other for $i\text{PrMgCl}$ and sulfur. The 1,2-ethanedithiol procedure resulted in a methanethiol group as well as a thiol group in place of the iodine. The other procedure resulted in the desired product as well as starting material. The $i\text{PrMgCl}$ and sulfur procedure was carried out on a larger scale from the first reaction and was closely monitored for completion. Through MALDI- TOF analysis it was found that the reaction was quenched by a sulfur impurity. Ways to get dry sulfur by recrystallization was researched and further testing was required.

STUDYING SYNUCLEINOPATHY IN REM SLEEP BEHAVIOR DISORDER TO FURTHER ADVANCE INTERVENTION RESEARCH FOR PARKINSON'S DISEASE

Sarah Ponder, Senior, Chemistry, University of Kentucky

Daniel Lee, School of Medicine, Kentucky Neuroscience Institute, University of Kentucky

Abstract:

Idiopathic REM sleep behavior disorder (RBD) is a powerful prodromal marker of neurodegenerative disorders defined by synucleinopathies, such as Parkinson Disease (PD), Dementia with Lewy Bodies (DLB), and Multiple System Atrophy (MSA). Characterized as the loss of REM sleep paralysis, over 80% of patients with RBD will develop neurodegenerative synucleinopathies. A protein believed to be at the center of PD and Lewy Body pathogenesis is Alpha-Synuclein (a-syn). Evidence suggests toxicity in affected cells is due to prefibrillar species, particularly large oligomers. Oligomeric a-syn has been shown to impair protein degradation, mitochondrial and endoplasmic reticulum function, and can also spread between cells, propagating disease. Found to be in the saliva and blood of PD patients, a-syn is readily available in non-invasive sample quantities. Patients chosen for the study will be accessed for RBD and age-matched controls to assess biomarkers for PD at longitudinal points in time. Other high-risk clinical factors include motor dysfunction, anosmia, color vision dysfunction, and cognition. Using ELISA and protein-based cyclic amplification methods of a-syn quantities, the goal is to determine the correlation of protein-based biomarkers with other high-risk clinical factors.

Chloe Porter, Senior, Chemistry, University of Kentucky
Beth Guiton, Chemistry, University of Kentucky

Abstract:

This research looks at how gold particles move and coalesce on a layer of graphene under the excitation of an electron beam. Several different sizes of particles were observed, and the phenomenon associated with each interaction between particles was recorded; this includes single-atom diffusion or a more abrupt snap-on effect between particles. To quantitatively understand the data, the radii were measured for each particle involved in the phenomena mentioned, and it was hypothesized that a larger difference in particle radii favored the occurrence of a snap-on effect. Therefore, above a certain threshold difference in radii, the particles would not diffuse or coalesce but rather the smaller of the two would abruptly jump to merge with the larger particle when energy was sufficient. At this point, more analysis is needed to support the hypothesis.

SYNTHESIS OF CYCLOMETALATED GOLD (III) COMPOUNDS**Libby Ratliff, Junior, Chemistry, University of Kentucky**

Samuel Awuah, Chemistry, University of Kentucky

Sailajah Gukathasan, Chemistry, University of Kentucky

Abstract:

Cancer is one of the deadliest diseases in the world and specifically in the United States. There is no perfect cancer treatment as many of them include intense side effects that disrupt patients' lives. Gold (III) based metallodrugs were synthesized in this experiment to be further tested in treating tumors. Five various cyclometalated gold (III) compounds were synthesized with five different ligands, totaling to twenty-five compounds attempted to be synthesized. After further analysis it was determined the compound composed of a phosphine ligand reacted with a carbonyl gold (III) was the most viable in vivo and efficient at tumor reduction. This compound's purity was verified via proton NMR and a crystal structure was grown. Biological studies were conducted with the carbonyl gold compound including cell cycle, cell viability, and apoptosis tests to reveal the stability of the structure and how lethal it is. Further testing must be done to determine the mechanism of action of the compound and how effect the compound is in reducing tumor size.

**ROOM TEMPERATURE SYNTHESIS OF POLYMERIC SULFIDES
BASED ON PYROMELLITIC DIIMIDES**

Jessica Ray, Senior, Chemistry, University of Kentucky

Mark Watson, Chemistry, University of Kentucky

Abstract:

Poly (arylene sulfide)s were prepared under mild conditions at room temperature by exploiting the highly electrophilic nature of core-halogenated pyromellitic diimides (PMDI), incorporating the PMDI units into polymer backbones via nucleophilic aromatic substitution with thiolate nucleophiles. The PMDI units are incorporated along their short axes, as opposed to traditional polyimides. One PMDI substitution pattern leads to an unusual solubility trend in halogenated solvents suggesting host-guest interactions. As a result of the sulfide groups being good nucleophiles and leaving groups, the polymers can be depolymerized to their monomeric species with excess monothiolate, insinuating potential renewability. This research project was completed in the University of Kentucky's CHE 533 capstone organic chemistry laboratory course.

SYNTHESIZING A SINGLE-ATOM CATALYST TO IMPROVE THE EFFICIENCY OF PEM FUEL CELLS

Jenna Rector, Junior, Chemistry, University of Kentucky

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Abstract:

Due to the rising concentration of atmospheric carbon dioxide (CO₂) from burning fossil fuels, finding clean alternatives for energy conversion is imperative. Fuel cells are a solution to this problem; however, the catalysts that are currently used in fuel cells have certain limitations. If we can overcome these limitations by synthesizing a new catalyst, the fuel cell will be an efficient, cost-effective form of sustainable energy which can be used on a global scale. Replacing non-renewable energy with fuel cells to power industrial buildings, residences, cars, and other forms of transportation will reduce the atmospheric CO₂, leading to a safer and more sustainable environment.

Polymer electrolyte membrane (PEM) fuel cells contain a cathode, where an oxygen reduction reaction (ORR) occurs. This reaction limits the efficiency of the fuel cell because it is nonspontaneous, thus requiring a catalyst for activation. Typically, fuel cells use catalysts synthesized from platinum nanoparticles, but these catalysts are expensive and unstable due to the use of precious metals and the surface-level attachment of the catalyst to the carbon nanodot (CND).

The purpose of our experiment was to synthesize a single-atom catalyst (SAC) in order to combat these limitations. We used bottom-up synthesis starting with citric acid (CA). We first melted the CA to loosen the carbon-carbon bonds, then added deionized water and a solution containing a transition metal. Next, we placed the solution in the hydrothermal reactor to heat stabilize the metal-ligand complex. After heat stabilization, we used pyrolysis to incorporate the metal-ligand complex into a graphene structure, before grinding this product and using it to make ORR ink. The key to success in this project was understanding and controlling the formation of this metal-ligand complex. This experiment resulted in a successful SAC incorporated in a CND, which shows promise of increasing efficiency of fuel cells.

USE OF BENZYLIDENE FOR THE SYNTHESIS OF A KEY GLUCOSIDE INTERMEDIATE

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Abstract:

The small molecule inhibitor, ipomoeassin F (ipo-F) is of great interest because of its ability to inhibit cancer cell growth. Ipo-F functions by blocking the subunit $\text{sec61}\alpha$, which is in the endoplasmic reticulum (ER) membrane. This blockage in-turn prevents proteins from entering the ER lumen where they would mature, which leads to cell death. We have been synthesizing analogues of ipo-F to maximize its function against various cancer cell lines. However, to do this more efficiently we are first optimizing the seven-step synthesis of the glucosyl donor (a key intermediate in the synthesis of ipo-F) by utilizing benzaldehyde dimethyl acetal instead of 2,2-dimethoxypropane. The thought process behind this change is would the aromatic ring make the structure more stable and easier to cleave later in the synthesis? If this change effectively simplifies the synthesis of the intermediate molecules, as well as the removal of the protecting group we will be able to enhance ipo-F's function against cancer cell lines.

SYNTHESIS OF SILVER NANOPARTICLES BY CHEMICAL REDUCTION METHOD: EFFECT OF REDUCING AGENT AND SURFACTANT CONCENTRATION

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Abstract:

Uniform, well-dispersed, silver nanoparticles (AgNPs) were prepared by a simple chemical reduction method. The particles were synthesized via the reduction of AgNO_3 by trisodium citrate and ascorbic acid as a surfactant. The resulting AgNPs were characterized by X-ray diffraction analysis, transmission electron microscopy, and scanning electron microscopy. It was found that the size of the AgNPs ranged from 35–80 nm, with an average of 50 nm. In this study, the effects of trisodium citrate and ascorbic acid, which act as reducing agent and surfactant respectively on the morphology of the silver nanoparticles, were investigated. It was found that the increasing concentration of trisodium citrate resulted in decreasing size of silver nanoparticles, while increasing the concentration of ascorbic acid shows the opposite effect. Moreover, the quasi-spherical shape of as-synthesized silver nanoparticles is also more uniform with the increase of trisodium citrate. Meanwhile, a slight change in particle shape from quasi-spherical to polygonal was observed as the concentrations of ascorbic acid were increased..

INVESTIGATION OF OPTIMIZED SYNTHESIS CONDITIONS FOR TEREPHTHALATE PRODUCTION

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Abstract:

Although the Claisen Condensation of diethyl succinate has documented use as an instructional tool for undergraduate organic chemistry, our work replicating the reaction under various conditions produces an alternative tautomer to that reported in the literature. Throughout our investigation of the tautomerization, we discovered 2,5-dihydroxyterephthalate as a by-product of the reaction. Our work focused on conducting the Claisen Condensation under various conditions (e.g., solvent, temperature, work-up, time, inert environment) with the goal of developing a better understanding of the tautomeric equilibrium, investigating potential aggregation, and optimizing the synthesis of the terephthalate derivative. This would allow our work to provide a potentially greener route to terephthalic acid (a reagent relevant to the production of PET plastic), while also establishing a multifaceted undergraduate procedure that accurately depicts the product of the Claisen-Dieckmann Condensation of diethyl succinate.

NICKEL TUNGSTATE DOPED WITH TRANSITION METALS FOR PHOTODEGRADATION OF ORGANIC COMPOUNDS

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Abstract:

Nickel tungstate semiconductor nanomaterials have shown their applications in energy conversion and photodegradation of organic dyes owing to its low band gap, high mechanical stability and abundant oxygen sites for dye molecule absorption. Nanoparticle nickel tungstate doped with different transition metals has been synthesized by co-precipitation methods with thermal treatment. Synthesized samples were examined using X-ray diffraction (XRD), transmission electron microscopy (TEM), dynamic light scattering (DLS) and X-ray photoelectron spectroscopy (XPS) methods. A series of photodegradation reactions were performed to assess the change in efficiency based on the doping metals (Fe, Co, Cu, Zn) and doping level of the samples. We find that doping tends to improve photodegradation rates, while the effect is different for each type of dopant. Theoretical calculations were also performed to investigate the electronic effects of doping and the nature of the valence band edge and conductance band edge.

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OPTIMIZATION AND MECHANISTIC INSIGHTS OF THE ALLYLATION OF PHENOLS WITH ALLYLOXYPYRIDINIUM TRIFLATE

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Philip Albiniak, Chemistry, Ball State University

Abstract:

2-allyloxy-1-methylpyridinium triflate (AOPT) was first developed in 2015 as an effective reagent for the allylation of carboxylic acids under mild conditions. Since that time, the Albiniak group has continued investigating the reactivity of AOPT with other nucleophiles. This presentation will focus on the reactivity of AOPT with phenols. Since these compounds are less acidic than carboxylic acids, a key component of this investigation will be examining a series of basic additives to the reaction mixture. In addition, a variety of variables including solvent, temperature, concentration, and reaction volume will be investigated. Interestingly, the size of the reaction vessel appears to be a critical component for the success of this allylation reaction. This observation may provide meaningful insight into the mechanism of allylic transfer in these reactions, and could help clarify the details of the substitution process for oxypyridinium salt reagents generally.

DEVELOPMENT OF NOVEL CARBONIC ANHYDRASE BIOMIMETIC ZN-METAL COMPLEXES FOR THE CATALYSIS OF CO₂ HYDRATION IN POST-COMBUSTION CARBON CAPTURE SYSTEMS

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Abstract:

To minimize the effect industry has on climate change, post-combustion carbon capture methods are being implemented to reduce carbon dioxide (CO₂) emissions. CO₂ has been strongly correlated as a driving force of anthropogenic climate change making the development of post-combustion carbon capture methods potentially important to lower atmospheric CO₂ concentration. The focus of this project to date has been the design, synthesis, characterization, and testing of novel catalysts for CO₂ hydration, a common reaction used in post-combustion carbon capture systems, which are typically based off amine or caustic solvents. These novel Zn-metal complexes were based off the binding site of carbonic anhydrase (CA), an enzyme that catalyzes CO₂ hydration in biological systems. Although not a novel concept, this project seeks to improve on popular synthetic CA active site mimics by more accurately replicating the metal-ligand bond angles present in CA by using a rigid cyclohexane-based ligand. Augmentations of the original novel Zn-metal complex are underway to improve organic solubility by the addition of an n-butyl chain and iso-butyl groups to the original ligand. Initial testing of the original Zn-metal catalyst was conducted via pH studies. Characterization of the original Zn-metal complex was completed by nuclear magnetic resonance (NMR) spectroscopy and elemental analysis while intermediates during the synthesis of all Zn-metal complexes were characterized by NMR spectroscopy.

A NOVEL FLAVOR-PAIRING TOOL TO CREATE NEW CRAFT BREWS IN THE BEVERAGE INDUSTRY

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Li Li Zyzak, Chemistry, Eastern Kentucky University

Abstract:

Food and beverages are necessities of life and consumer goods companies dedicate significant resources to develop innovative concepts that consumers prefer. In a space where consumer has few choices, it's easy to understand why they prefer one brand over the other. However, as category options expand it becomes more challenging. This is the case in the craft brew industry. In 2018, beer sales decline 1% while the craft brew sales volume grew 4% reaching 13% of the total beer market by volume¹. Craft brews are sold at a higher premium and accounted for \$27.6 billion in 2018, 24% of the \$114.2 billion US beer market¹. One of the biggest challenges for craft breweries is the ability to continue developing new taste perceptions. The goal of our project is to utilize science to develop an algorithm and blending tool enabling the user to create new and interesting flavor concepts for the craft brew industry. We leveraged the science of linking important flavor compounds from craft brews with similar flavor compounds in other food products. The uniqueness of our approach is two-fold: (1) we placed weighing factors (multipliers and rankings) on the flavor compounds in the food products, (2) we have created a flavor wheel description to aid in the user-friendliness of the tool. Our tool will provide a simpler and cost effective prototyping device for creation of new flavors for the brewing industry.