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2013 Oklahoma Research Day

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05. Chemistry

University of Central Oklahoma

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Abstracts from the 2013 Oklahoma Research Day

Held at the University of Central Oklahoma

05. Mathematics and Science

05. Chemistry

05.05.01 Synthesis and Characterizations of Platanum Coordinated Thiophene and Thiolate Complexes

Dr. A.K. Fazlur Rahman,

Oklahoma School of Science and Mathematics

Abstract: In our contuning effort to develop platinum based hydrodesulfurization catalyts we have synthesized a series of platinum bound thiophene and thiolate complexes. We have spectroscopically characterized complexes (I, II, III) obtained from the reaction of $(C_6F_5)_2Pt(THF)_2$. We have also synthesized a series of thiolate complexes by reacting DialkyPtatinumcyclooctadeine with various thiols to produce thiolato complexes via classical oxidation addition and reductive elimination mechanism. X-ray crystal structure of these complexes will be compared and a possible mechanism will also be suggested.

05.05.02 SPEME GCMS Method for the Analysis of Triclosan in Sewage Treatment Outflow Waters

John Bowen, Al Albahadily, Alex Matunas, Billy Frenier, Gregory Melsby, Kaci Rosales,

University of Central Oklahoma

Compounds including drugs, and environmentally or medically deliterous are concentrated into the sanitary sewage treatment plants and some fraction is released through the outflow waters into local streams. An analytical method for the analysis of a model drug compound Triclosan was developed and tested. The method was then used to quantitate triclosan from two treatment plant outflow waters.

05.05.03 Development of a Paper-Based Biosensor for Antibodies in Serum

John Bowen, Barry Lavine, Mary Tappert, Nicolas Shaffer,

University of Central Oklahoma

A test biosensor for antibodies in serum based on the microfluidic Paper-Based Analytical Device (μ -PAD) pioneered by the Whitesides Group (Chemistry, Harvard University) was developed to detect and identify anti-Bovine Serum Albumin (anti-BSA) using BSA immobilized onto the cellulose of filter paper. The biosensor μ -PAD used wax microfluidic channels and the familiar BCIP/NBT microspot color change reaction for the detection scheme. After the complete testing of this test biosensor, a biosensor μ -PAD will be produced to detect antibodies in sheep blood generated in response to two viral diseases Epizootic Hemorrhagic Disease Virus (EHDV) and Blue Tongue Virus (BTV).

05.05.04 Development of Hybrid Format Upper-Level Chemistry Course

Joel Smith,

Southeastern Oklahoma State University

Alternative delivery methods to the traditional face-to-face college lecture have become a fixture in higher education. A hybrid delivery format course was developed and piloted for quantitative analysis (Chemical Analysis) at Southeastern Oklahoma State University in the Fall 2012. The hybrid format consisted of 2-3 hours of video lectures and one hour of traditional face-to-face meeting weekly. Video lectures were recorded using a SmartBoard and microphone which were then converted to a format suitable to be viewed on any computer or handheld device including smartphones. Video lectures are uploaded to a server and linked to the Blackboard page. Overall student performance will be compared to previous years using traditional face-to-face format. Statistics of student access to the video lectures will be discussed. A student survey of the piloted format will be present with student suggestions for improvement.

05.05.05 Computation of Solvent Effects on Energetics of Metallocene-Catalyzed Ethylene Polymerization

Paritosh Das, Emvia Calixte,

Cameron University

Computationally, we have investigated the effects of several solvents (namely, cyclohexane, toluene and dichloromethane) on the energetics of various steps of metallocene-catalyzed ethylene polymerization. $[\text{CpCH}_2\text{Cp}]\text{ZrR}^+$, with $\text{R} = \text{CH}_2\text{CH}_2\text{CH}_3$ have been primarily used as the model active catalyst species. For comparison purpose, some computational data have also been obtained on catalyst systems bearing F and CH_3 substituents on the Cp ligands. All calculations were based on density functional theory (DFT/B3LYP). Compared to the gas-phase, the solvents are found to stabilize the individual cationic species (namely, reactants, products, intermediates and transition states) significantly. However, these effects largely cancel each other when applied to specific reaction steps (except for steps such as complexation or product separation for which the reactant or the product is a cation of the form $[\text{CpCH}_2\text{Cp}]\text{ZrR}^+$).

05.05.06 Dihydrodipicolate Synthase from E. coli: Mutagenesis of Threonine 44 to Valine

Russell Evans, Lilian Chooback, Yvonne Daugherty,

University of Central Oklahoma

Dihydrodipicolate Synthase (DHDPS), an enzyme in plants and bacteria, is a component of the L-lysine biosynthesis pathway. DHDPS catalyzes the first committed step in this pathway. The first committed step in the pathway is the reaction of pyruvate and L-aspartate- β -semialdehyde (ASA) to produce dihydrodipicolinate. L-lysine, the final product of the pathway, inhibits DHDPS. Previous literature has shown that DHDPS follows the ping-pong kinetic mechanism. In the first step in this pathway, the ϵ -amino group of Lysine161 places a nucleophilic attack on the carbonyl of pyruvate, producing a Schiff base. The Schiff base intermediate undergoes an irreversible dehydration step and forms an enamine intermediate. Next, ASA binds to the enzyme- enamine complex. Threonine 44 is located on the boundary of the active site of DHDPS. It is proposed that threonine 44 is involved in a proton shuttling process into and out of the active site. To determine the role of threonine 44, site-directed mutagenesis was carried out to develop the T44V mutant. To characterize the T44V mutant enzyme, kinetic studies will be performed. This work was supported by grant P20RR016478 from the National Center for Research Resources a component of the National Institutes of Health and a grant from the University of Central Oklahoma Office of Research and Grants.

05.05.07 Soil Conductivity Analysis of the Formation and Detection of Perchlorate Brines on Mars

Kayla Love, Laura Fernandez, Vincent Chvevri,

Langston University

The deliquescent property of perchlorates may play a role in controlling Martian soil and atmospheres water content on Mars. Moreover, research supports ambient air moisture contributes to the formation of liquid water on Mars's surface. My goal was to develop a technique to enhance detectability of perchlorate brines on Mars. To achieve this, we focused on electric conductivity of perchlorate brines during the liquidus phase where both liquid water and perchlorate are stable indicating the deliquescence limit. Palaganite Soil (JSC Mars 1), which is most similar to regolith found on Mars, was used with various concentrations. JSC Mars 1 samples were in closed environments surrounded with water to ensure 100% relative humidity and kept at approximately 73°C. Copper electrodes, attached to a micrometer, were inserted into samples. Samples were kept in closed environments surrounded with water to ensure one hundred percent relative humidity and kept at approximately 73°C. To observe conductivity of samples, amount of resistance was recorded over time. Results illustrated that recorded resistance and concentration of $(MgClO_4)_2$ were inversely proportional. Learning more about the behaviors of perchlorates in a Martian environment will expand research on the past conditions, current conditions, potential for biological life, and preparations for human explorations on Mars.

05.05.08 Fabrication and Characterization of a Solid State of Organic Photovoltaic for the Purpose of Improving Efficiency

Dane Scott, Cody Soden, Joshua Smith, Laura Blanco-Berdugo,

East Central University

Solid State Organic solar cells are of interest because they are less expensive, can be fabricated by rolling or printing processes and made of renewable materials. However, low efficiency prevents mainstream use. This work examines the possibility of using charged layers in the solid state matrix of the solar cell in order to improve electron pair separation leading to improved efficiency. The cells have been constructed using a 100 nm Al anode with a conductive polyacrylonitrile electrolyte and connecting to that a 14 ohms/square ITO slide with calcinated TiO₂ which was dye sensitized with Copper Phthalocyanine. Cells were also constructed in which the conductive electrolyte layer was treated with HCl and PDDA. Both cells were illuminated using a 1.5 AM solar simulator and characterized using the Amprobe 600 Solar Analyzer.

05.05.09 Characterization of the Slow-Binding Inhibition by Acetopyruvate of the Dihydrodipicolinate Synthase from E. coli

Lilian Chooback, Priscilla Seabourn, William Karsten,

University of Central Oklahoma

Dihydrodipicolinate synthase (DHDPS) catalyzes the first step in the biosynthetic pathway for production of L-lysine in bacteria and plants. The kinetic mechanism is ping pong with pyruvate binding to free enzyme and L-aspartate-b-semialdehyde (ASA) binding to the F enzyme form. The enzyme is feedback inhibited by the end-product L-lysine. The enzyme has received interest as a potential drug target since it is not present in mammals. Acetopyruvate is a slow-binding inhibitor of DHDPS competitive versus pyruvate with an initial K_{is} of about 25 mM and a final inhibition constant of about 4 mM. The enzyme:acetopyruvate complex displays an absorbance spectrum with a λ_{max} at about 303 nm and a longer wavelength shoulder. The rate constant for formation of the complex is 0.03 s⁻¹. The enzyme forms a covalent enamine complex with the first substrate pyruvate and can be observed spectrally with a λ_{max} at 275 nm. The spectra of the enzyme in the presence of pyruvate and acetopyruvate shows the initial formation of the enamine intermediate followed by the slower growing in of the E:acetopyruvate spectra with a rate constant of 0.005 s⁻¹. The enzyme is proposed to form a covalent Schiff base between acetopyruvate and K161 on enzyme that subsequently deprotonates to form a resonance stabilized anion similar to the enamine intermediate formed with pyruvate.

05.05.10 Analysis of Oklahoma mushroom fruiting-body odors using GCMS and Solid Phase Microextraction

John Bowen, Alex Matunas, Clark Ovrebo, Kaci Rosales,

University of Central Oklahoma

Various mushrooms including varieties of stinkhorns use a reproductive strategy involving disagreeable odors to disseminate their spores by drawing flies. In this study, an analytical method using Gas Chromatography Mass Spectrometry and Solid Phase Microextraction was developed to analyze the odor causing compounds of *Lysurus mokusia* and other wild mushrooms. Results from four species of stinkhorn mushrooms will be presented and the compounds identified in each species will be compared.

05.05.12 Indigo Blue: Connecting its Chemistry with History

Dene Betz, Caleb Wood, Dr. A.K. Fazlur Rahman, Ethan Wood,

Oklahoma School of Science and Mathematics

This presentation illustrates the intriguing connection of the chemistry of Indigo blue and its history in the context of chemical synthesis and agricultural production centuries ago in British India. Indigo blue was cultivated in India for almost two hundred years. It started about 1780 and continued until World War I. Von Baeyer, a German Chemist synthetically produced Indigo blue in 1890, and it was not heavily commercialized until 1913. The agricultural production of Indigo in India has its own story. From the confiscation of agricultural land to an extensive labor oriented extraction process, indigo production took a human toll. The natural extraction process, the laboratory synthesis and its usage in the past and present are described in this presentation.

05.05.13 GC/MS Comparison Analysis of Wormwood Related Plants Serving as a Natural Way of Deworming Farm Animals Versus Current Deworming Products.

Megan Meek, Tiffany Maher,

Northeastern State University

The increased utilization of natural resources is a growing trend among farm owners. The term "going green" doesn't only help the environment, but it also helps many farmers substantially when it comes to controlling costs. Wormwood is an herb commonly used for farm animals to treat worm infections. Common ragweed, giant ragweed and *Sesuvium portulacastrum* are all relatives to wormwood that grow naturally in Oklahoma. The primary objective is to be able to use these natural growing plants as a dewormer for farm animals in place of deworming products currently on the market. The composition of hexane and ether extracts from branches, leaves and blooms of each were investigated. Samples were analyzed using GC/MS and compared against ivermectin, fenbendazole and moxidectin.

05.05.14 Transition Metal Binding by Desferrioxamine

Brianna Broad,

Northeastern State University

Desferrioxamine (DFO) is one of the most well-characterized microbial siderophores. In this study a series of metal ions were evaluated for binding by DFO. Solutions of DFO were titrated with Fe(III), V(II), Co(II), Ru(III), Ga(III), or Mn(II) in a buffered solution at room temperature. Metal ion binding was monitored using a UV-VIS spectrophotometer, scanning from 700 to 200 nm, after incubating the solutions of siderophore and metal for at least 20 minutes. Iron, Vanadium, Cobalt and Ruthenium were bound by DFO under the experimental conditions. Gallium and Manganese were not bound by DFO under these conditions. The next set of experiments will evaluate the strength of binding through competition and by determination of formal binding constants.

05.05.15 Identifying Ada City Water Leaks by Measuring Ca, Mg, and Total Hardness

Destiney Shouse,

East Central University

The source of the Ada, OK water supply is Byrd's Mill Spring which comes from the Arbuckle Simpson aquifer. The calcium to magnesium to hardness ratios in this aquifer have been shown to be consistent over time (1) and can serve in distinguishing water pipeline leaks from natural seeps throughout the city. Water samples were collected and analyzed for calcium and hardness to determine their source. The initial plan called for sampling in the Ada metropolitan area to distinguish natural seeps from Ada city water with the use of two USEPA titrimetric methods. This plan was modified due to difficulty with the calcium procedure and the summer drought. The results clearly showed the distinction between Ada city water and samples from other sources.

05.05.16 The Synthesis and Reactivity of a NNC Nickel Chloride Complex

Steven Meier, Amanda Purcell, Jessica Laverty, Kelsey Coy,

University of Central Oklahoma

The NNC ligand (NNC = 6-phenyl-2,2'-bipyridine) has been cyclometallated to palladium, platinum, iridium, and rhodium to generate a variety of complexes that are capable of cleaving the C-H bond. Edwin Constable who originally synthesized the NNC ligand was able to attach the ligand to platinum and palladium, but no results were reported on using nickel. The NNC ligand is normally attached to transition metals through insertion of the metal into the aryl C-H bond. However, this route was not successful for the attaching the NNC ligand to nickel. It is widely known group 10 metals insert into aryl halide bonds, and this was exploited in the synthesis of the NNC nickel complex. The NNC halide derivative 6-(2-chlorophenyl)-2,2'-bipyridine was synthesized and attached to nickel through insertion using bis(cyclooctadiene)nickel(0). The resulting (NNC)NiCl complex is sparingly soluble in chloroform, therefore, an alternative ligand 6-(2-chlorophenyl)-4-(p-anisole)-2,2'-bipyridine was synthesized and attached to nickel. Work has been ongoing to replace the chloride ligand with various other ligands such as phenyl, ethoxide, and trifluoroacetate in order to generate a more reactive complex.

05.05.17 The Synthesis of a Ruthenium NNC Pincer Complex

Steven Meier, Luis Figueroa,

University of Central Oklahoma

The NNC ligand (NNC = 6-phenyl-2,2'-bipyridine) has been cyclometallated to palladium, platinum, iridium, and rhodium to generate a variety of complexes that are capable of cleaving the C-H bond. Edwin Constable who originally synthesized the NNC ligand was able to attach the ligand to a ruthenium terpyridine complex, but that complex was not able to be used as a C-H activation catalyst. The goal of this research has been to try to develop other ways to attach NNC derivatives to ruthenium in order to produce a C-H activation and functionalization catalyst. The NNC ligand is normally attached to transition metals through insertion of the metal into the aryl C-H bond. However, this route has not been successful for the synthesis of the ruthenium NNC complex. Therefore, alternative routes had to be developed. Others have shown that the easily synthesized $(\text{Ph}_3\text{P})_3\text{RuCO}(\text{H})_2$ complex, after reduction to ruthenium(0), inserts into aryl bromide and aryl iodide bonds. Several other NNC halide derivatives have been synthesized, and work has been ongoing to insert ruthenium into the aryl halide bond in order to attach the NNC ligand to ruthenium. Future work will be focused on modifying the (NNC)ruthenium complex into an active C-H activation catalyst.

05.05.18 Dynamic Coupling of Rotors and Axles in Rotaxanes

James Dechter, Kim Pham, William Garbe,

University of Central Oklahoma

Supramolecular structures are held together by intermolecular forces rather than chemical bonds. They are of interest for purposes ranging from the construction of the various components of molecular machines in nanotechnology, to the study of the self-assembly of molecules. Our interest in nuclear magnetic resonance (NMR) studies of the dynamic coupling of supramolecular structures has led us to investigate "rotaxanes", which derive their name from their description as a rotor molecule threaded onto an axle molecule. Our interest is to probe the effect of the diameter of the rotor molecule on the dynamic behavior of the axle molecule – an effect called dynamic coupling. We have chosen a series of cyclic polymers as the rotors which have the common name cucurbiturils. The series with 5-8 monomer units are commercially available, and the specific polymer is designated by the n in cucurbit[n]uril. The axle we have chosen is spermine tetrahydrochloride ($\text{SPM}\cdot 4\text{HCl}$). Evidence will be given for the formation of rotaxanes between the axle $\text{SPM}\cdot 4\text{HCl}$ and the two rotors, cucurbit[6]uril and cucurbit[7]uril. Preliminary results for the dynamic coupling experiments for these systems will be presented. Also, we will present evidence confirming the formation of a charge-transfer complex in the interior of the cucurbit[8]uril rotor when methylviologen and hydroquinone are used together as rotors.

05.05.19 Reversed Phase HPLC Analysis of B-Vitamins

Stormie Holcomb, Jessica Martin,

Northeastern State University

B-vitamins are a very important part of the human system. B-vitamins are found in most multivitamin tablets. A lack of certain B-vitamins can cause diseases, such as a deficiency of folic acid can cause anemia. For our research, we followed a simple HPLC reversed phase system that provides analysis of certain B-vitamins using an Ascentis Express C18 column from Sigma Aldrich. The purpose of this experiment was to develop a method for analysis of folic acid, pyridoxine, and thiamine hydrochloride using HPLC to ultimately test multivitamin tablets and verify the amount of the B vitamin contained in the product or test the degradation of the vitamin over time. A reversed phase HPLC method was developed and a standard curve was created for each B-vitamin. The method developed can be used in the future to analyze the content of these B-vitamins in various supplements.

05.05.20 Synthesis and Evaluation of a New Generation of Highly Acidic Nucleophilic Glycine Equivalents for the Preparation of Unnatural α -amino acids

Trevor Ellis,

Southwestern Oklahoma State University

A series of highly acidic nucleophilic glycine equivalents, valuable for the preparation of unnatural α -amino acids via homologation approaches, have been developed. These novel nucleophilic glycine equivalents are founded on the modular design of Ni(II) glycine Schiff Bases. The increased acidity of the α -protons of the glycine moiety arises from the strategic introduction of trifluoromethyl group(s) into the benzophenone module of the nucleophilic glycine complexes. The syntheses of the various trifluoromethyl containing glycine equivalents, as well as the previously unreported synthesis of the necessary trifluoromethylated amino-benzophenones, are described. The reactivity of this series of glycine equivalents has been investigated by the evaluation of competitive reactions between the Ni(II) complexed glycine equivalents containing a 2-aminobenzophenone, a 2-amino-4'-(trifluoromethyl)-benzophenone, or a 2-amino-3',5'-bis(trifluoromethyl)-benzophenone moiety under kinetic or thermodynamic reaction conditions.

05.05.21 Nutritional Benefits of Different Tomato Strains: A Look at Glucose, Fructose and Vitamin C.

Tyler Vann, Lilian Chooback,

University of Central Oklahoma

Depending on the strain and freshness, the nutritional content of tomato may vary. Using anthrone reagent the total concentration of carbohydrates in the tomato can be measured. The anthrone dehydrates monosaccharides to form furfural derivatives. The formation of the furfural derivatives were evident by appearance of brown color and the intensity of the color was proportional to the concentration of fructose. To distinguish between glucose and fructose the sample was exposed to resorcinol, which reacts much quicker with ketoses as compared to aldoses. Using spectroscopy and monosaccharide standard the glucose and fructose content of different tomato sample were found. It was discovered that the Grape and Romano strains had a higher concentration of fructose when compared to the Cluster and Campari strains. We are in the process of measuring the ascorbic acid contents of the same tomato samples using test strips.

05.05.22 Dihydrodipicolinate Synthase From E. coli: Site-Directed Mutagenesis of Arginine 138 and Lysine 133

Tyler Vann, Charles Nguyen, Lilian Chooback, William Karsten,

University of Central Oklahoma

Dihydrodipicolinate synthase catalyzes the formation of dihydropicolinate from pyruvate and L-aspartate-R-semialdehyde(ASA). The enzyme catalyzes the first committed step for the biosynthesis of L-lysine in bacteria and plants. The enzyme from Escherichia coli is feedback inhibited by lysine, the end product of the pathway. A study of the pH dependence of the kinetic parameters was done to elucidate the acid-base chemical mechanism of the enzyme. The Σ -amino group of lysine 161 attacks the carbonyl of pyruvate and forms a Schiff base intermediate. The loss of a proton from this intermediate leads to the formation of an enamine intermediate. The second substrate, ASA binds to the enzyme:enamine covalent intermediate. Site-directed mutagenesis was done to investigate the role of the active site arginine 138 (R138), and lysine 133 (Y133). The R138A, R138K, and Y133F mutants were created and the identity of the mutants was confirmed by DNA sequencing. Kinetic studies will be done to characterize the mutant enzymes. This work was supported by grant P20RR016478 from the National Center for Research Resources a component of the National Institutes of Health and a grant from the University Central Oklahoma.

05.05.23 Biomass Deconstruction to Produce Sugars Using Ionic Liquid

Jude Abia, Rashad Ismayilov,

Northeastern State University

The ability to use cellulosic biomass for the large scale production of fuels and chemicals depends critically on the development of effective conversion processes. The major technological barrier to using cellulosic biomass has been the depolymerization step in which sugars are produced for conversion into molecules with higher energy densities than the parent biomass. The high energy cost and difficulty in processing biomass are the main roadblocks to the widespread commercialization of this renewable energy source. We report on the development of technologies involving ionic liquids that can i) efficiently deconstruct cellulosic biomass to release cellulose and hemicellulose, ii) hydrolyze cellulosic components to produce sugars.

05.05.24 Conversion of Vegetable Oil to Biodiesel Using Microwave Irradiation

Tyler Scott, Spence Pilcher,

Northeastern State University

With the ongoing rise in cost of crude oil and focus on global warming, finding renewable energy sources is a current area of trending research. Biodiesel is an alternative energy source that has sparked interest in our region due to its ability to reduce toxic emissions, reduce dependence on foreign oil, and contribute to rural economic development. To introduce undergraduate research students to this topic, an experiment was developed for the organic chemistry II laboratory course which entailed preparing biodiesel from vegetable oil using microwave irradiation. The procedure that afforded the highest conversion of vegetable oil to biodiesel used potassium hydroxide as the catalyst (1.0wt% in methanol) and reacted at 50°C for 5 minutes.

05.05.25 Genetic Variation in PPAR γ at Nucleotide 1431 Impairs Obesity Related Phenotypes in Response to Exercise Training

Martell Mckinney,

Langston University

Obesity is now the second leading cause of death in the United States, and is likely to become the first. Exercise can significantly reduce body mass and decrease BMI, a measurement used to determine obesity. However, not all overweight patients respond suitably to exercise. Research supports a "possible" candidate gene that may affect responses to exercise training in obese patients: Peroxisome Proliferator-Activated Receptor Gamma (PPAR γ). PPAR γ activates certain genes in a fat cell, resulting in the storage or burning of fat. Changes in PPAR γ gene polymorphism may have potential functional effects. Thus, we chose to determine whether the C1431T polymorphism influences the response to aerobic exercise training. Polymerase chain reaction (PCR) was used to amplify only DNA segments with PPAR γ . PCR products were subjected to restriction digestion by HpyCH41V which cleaved at 5'-ACGT-3' which included nucleotide 1431 and allowed us to recognize PPAR γ nucleotide specific genotypes and polymorphisms via a DNA gel. Results demonstrated significantly lower post-exercise BMI scores for carriers of thymine at PPAR γ nucleotide 1431 in response to exercise training when compared to carriers of cytosine PPAR γ nucleotide 1431. Our data contributes to supporting PPAR γ as a promising candidate gene for therapeutic treatment against obesity.

05.05.26 Cellulosic Ethanol for Biomass Fuel

Justin Watts,

Northeastern State University

There are many scientists in numerous countries, including the United States, working on solving the world's energy crisis. Research is being conducted on different technologies including solar power, wind power, and biofuels. The subject of my research is a specific type of biofuel called cellulosic ethanol. Ethanol itself is a highly combustible fuel, it even has a higher octane rating than premium gasoline. However, this also means that most engines need a blend of ethanol and gasoline to function without potential harm unless it is an E85 approved vehicle. Given the potential decrease in fossil fuel consumption and separation from dependence on foreign oil I believe harnessing the potential energy from the cellulose found in plants and fungi could be the greatest development of this century. The problem lies with the inefficient methods and high cost associated with ethanol, along with the biomass feedstock issues. In this experiment we will show how cellulose can be broken down into glucose by the enzyme cellulase, and fermented to produce carbon dioxide and ethanol. Cellulase is actually a group of enzymes that hydrolyze the glycosidic linkage between the glucose monomers. Since there are many different enzymes and many different linkages, finding the right enzyme and feedstock may prove crucial to this research.

05.05.27 Structure Activity Relationship Studies to Improve Cancer Drugs

Dana Rundle, Caitlin Kriewall, Kelsie Magiera, William Carroway,

University of Central Oklahoma

The objective of this study was to evaluate twenty-six E series compounds prepared by Dr. K. Darrell Berlin of Oklahoma State University for further research as cytotoxic agents toward ovarian cancer cells. The E series compounds are structural optimizations to increase solubility while preserving the cytotoxicity of the heteroarotinoid, SHetA2. The E series compounds and SHetA2 are called flexible heteroarotinoids (FlexHets) due to structural flexibility gained by adding a flexible urea or thiourea linker region. SHetA2 has a known 10 μ M LC50 in ovarian cancer cell lines, but has no comparable effect on normal cells in culture. E series FlexHet cytotoxicity was compared to that of SHetA2 utilizing a cell proliferation assay in cell culture models using A2780 and SK-OV-3 human ovarian cancer cells. Five E series compounds showed cytotoxicity comparable to that of SHetA2. An evaluation of structural features in E series compounds that promote cytotoxicity versus those features that do not may lead to the development of improved heteroarotinoids for possible therapeutic intervention. Currently the synthesis of E1 is underway to generate an amount sufficient for further analysis of its intracellular effects, and other potent E series compounds will be synthesized. Further studies of E series compounds will be done by kinase assay, kinase inhibition, and Western blotting to examine which signaling pathways and proteins these heteroarotinoids act upon to induce cell death.

05.05.28 Effects of microwave irradiation on the free-radically initiated microemulsion polymerization of styrene

Brent Roberts, Spence Pilcher,

Northeastern State University

Microwave irradiation has been used to enhance various organic reactions, improving reaction times and yields. In this study, the effects of microwave irradiation, as compared to conventional heating, on the radically-initiated microemulsion polymerization of styrene were investigated using varying initiators, initiator weight percent, and surfactant. The free radical initiators potassium persulfate (KPS) and 2,2'-azobis(2-methylpropanimidine) dihydrochloride (V-50) were used at weight percents of 0.1 and 1.0% with either stearyl trimethylammonium chloride (STAC) or cetyl trimethylammonium bromide (CTAB) as the surfactant. Polymerizations using conventional heating generally had slightly higher percent conversions over those identical procedures using microwave irradiation. However, the reaction that consistently had the highest percent conversion was initiated by 1.0 wt.% V-50 with CTAB using microwave irradiation. Polymerizations using V-50 consistently produced the most polymer at 1.0 wt.% when compared to KPS. The majority of trials initiated by 0.1 wt.% of initiator failed to produce polymer. The two surfactants yielded similar percent conversions with other parameters being the same. The molecular weight of the formed polystyrene was approximately 2×10^6 g/mol regardless of reaction parameters, and polydispersity indices were 2.0-2.5. Both microwave and conventional heating produced polymer samples having glass transition temperatures of approximately 10

05.05.29 N-Substituted Polycyclic Aromatic Hydrocarbons as Models for Organic Switches

Dwight Myers, Daniel McInnes,

East Central University

N-substituted polycyclic aromatic hydrocarbons are proposed for use as organic solid state transistors or switches[1]. Simple molecules of this sort include phenazine and dibenzo[b,i]phenazine. Using these molecules as simple model compounds, we have begun an ab initio computational study of these compounds and the effect of electron withdrawing or donating groups in place of hydrogens on the aromatic rings. Calculations have been made for phenazine and dibenzo[b,i]phenazine and their corresponding polycyclic aromatic hydrocarbons anthracene and phenazine. Work in progress and future directions will be discussed. 1. Wu, Y., Yin, Z., Xiao, J., Liu, Y., Wei, F., Tan K. J., Kloc, C., Huang, L., Yan, Q., Hu, F., Zhang, H., and Zhang, Q., "Crystal Structure and Phototransistor Behavior of N-substituted Heptacenes, Appl. Mater. Interfaces 2012, 4, 1883-1886.

05.05.30 Microwave Synthesis of Ti- and Y-Doped BIMEVOX Compounds

Dwight Myers, Chandra Thapaliya,

East Central University

Oxide ion conductors such as the BIMEVOX series of bismuth vanadium oxides are proposed as solid electrolytes for Solid Oxide Fuel Cells (SOFC)[1]. These are synthesized by substituting small amounts of a different metallic ion for vanadium in $\text{Bi}_4\text{V}_2\text{O}_{11}$ to give $\text{Bi}_4\text{V}_{1-x}\text{Me}_x\text{O}_{11-3x/2}$. Microwave assisted synthesis of BIMEVOX phases can greatly speed reaction times[2]. We have prepared the titanium and yttrium doped BIMEVOX phases with $x = 0.1-0.3$. X-ray diffraction patterns indicate the formation of high purity products. The effects of degree of compaction and different crucible materials have been examined. 1. F. Abraham, J.C. Boivin, G. Mairesse, and G. Nowogrocki, *Solid State Ionics* 40/41 (1990) 934-937 2. Vaidhyanathan, K. Balaji, and K. J. Rao, *Chem. Mater.* 1998, 10, 3400-3404

05.05.31 A Study of Varied Dopant Levels in BIMEVOX Compounds by Microwave Synthesis

Dwight Myers, Joshua Smith,

East Central University

Oxide ion conductors such as the BIMEVOX series compounds have applications in electrolyte membranes for Solid Oxide Fuel Cells (SOFC) [1]. BIMEVOX compounds were synthesized by substituting a different metal ion for vanadium in $\text{Bi}_4\text{V}_2\text{O}_{11}$ to give $\text{Bi}_4\text{V}_{1-x}\text{Me}_x\text{O}_{11-3x/2}$. This study focused on manganese, silver, and gallium doped BIMEVOX phases with $x=0.1-0.4$. The microwave assisted synthesis method of BIMEVOX has proven to greatly decrease reaction times [2]. X-ray diffraction patterns indicate that the products are of high purity. FTIR analysis has also been performed to characterize the compounds. Compaction of materials and different crucible materials have also been examined. 1. F. Abraham, J. C. Boivin, G. Mairesse, and G. Nowogrocki, *Solid State Ionics* 40/41 (1990) 934-937 2. Vaidhyanathan, K. Balaji, and K. J. Rao, *Chem. Mater.* 1998, 10, 3400-3404

05.05.32 The Prospects of Biofuel in Oklahoma: An Educational Study

Nathan Jia, Dr. A.K. Fazlur Rahman, Jimmy Wu,

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Oklahoma's economy is primarily based on agriculture and has also been dependent on oil and natural gas for almost fifty years. The demand for clean and renewable energy alternatives to fossil fuels such as organically produced ethanol is rapidly increasing in both the United States and the world at large. Oklahoma has the resources to become a powerful contributor to meeting this demand, a competitor in the biofuel market not only nationally, but also globally. The integration of biofuel technology into a petroleum based energy sector will bolster Oklahoma's agricultural economy and increase our preparedness for future energy crises. Also noteworthy is the participation of universities and industries in biofuel research, which will bring breakthroughs in the development of new crop systems as well as a new sector devoted to increasing agricultural production. These developments have the potential to greatly benefit Oklahoma's economy by creating many new job opportunities in both urban and rural Oklahoma. The aim of this study is to increase our understanding of biofuel research initiatives in Oklahoma.

05.05.34 Measuring Temperature Dependence on Charge Organization in Ionic Liquids

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Room temperature ionic liquids exhibit substantial amounts of charge organization in the liquid phase. Charge organization plays a significant role in defining the properties of ionic liquids and there are several coordinated solvation shells localized around cations. A central goal of research in this field is characterizing the degree of charge organization in an ionic liquid and correlating those values to properties of the materials that make them attractive as solvents. We propose a cost-effective method for investigating charge organization in a family of 1-alkyl-3-methylimidazolium trifluoromethanesulfonate ionic liquids using simple FT-IR spectroscopic techniques. Charge organization of the ionic liquids is measured as a function of temperature with the proposed method. Increased temperatures should increase the thermal motion of the ions composing an ionic liquid, disrupting any long-range charge organization. Furthermore, longer alkyl side chains attached to the imidazolium ring are expected to frustrate charge organization and further decrease the level of observed charge organization. FT-IR spectroscopic measurements confirm both of these hypotheses.

05.05.35 The Effects of Microwave Irradiation on the Microemulsion Polymerization of Methyl Methacrylate

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Microwave irradiation has several advantages as a heating method for chemical reactions including shorter reaction times, less energy required, and uniform heating. The project focused on the specific effects that microwave irradiation had on different parameters in the polymerization of methyl methacrylate (MMA) in microemulsions which were formed using stearyl trimethylammonium chloride (STAC) or cetyl trimethylammonium bromide (CTAB) as the surfactant. Initiator, initiator concentration, and reaction time were varied and the percent conversion and properties of the resultant polymer were compared to their conventional heating analogs. Polymerizations using microwave irradiation had a higher conversion rate than conventional heating at the 5 minute reaction time and at lower initiator concentration (0.1 wt.% monomer). For longer reaction times and standard initiator concentrations (1.0 wt.%) the percent conversions from the two heating methods were similar. Reactions using 2,2'-azobis(2-methylpropionamide) dihydrochloride (V-50) achieved approximately 10% higher conversion rate on average than those employing potassium persulfate (KPS) as the initiator regardless of heating method. V-50 consistently produced polymer at a low concentration (0.1 wt% monomer) in the microwave. Latex particles sizes were 17-31 nm, molecular weights were 9.9×10^5 - 2.8×10^6 g/mol, and polydispersities were 1.6-2.2 and were independent of all parameters other than concentration.

05.05.36 Developing Laboratory Experiments for General and Organic Chemistry Labs Using the Vernier LabQuest

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Nalley, Department of Physical Sciences, Cameron University, Lawton, OK 73505 Recently the Cameron University of Physical Sciences purchase Vernier Lab Quest Data Collecting Devices and associated instrumentation and sensors in order to facilitate data collection in our chemistry and physics laboratories. LabQuest is a standalone and computer interface for Vernier sensors or other data collecting devices. It uses its color touch screen to collect, graph, and analyze data in the classroom or in the field. In this project we were interested in developing experiments using the Vernier Polarimeter which could be adapted to general, organic or biochemistry laboratories. The polarimeter can be used to measure chiral properties of optically active samples without chemically modifying or destroying the sample. This poster will describe three experiments which were developed for our laboratories using the Vernier Polarimeter.

05.05.37 Determining the Cause of Temporal Instability of Self-Assembled Gold Nanoparticle Thin Films

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Gold nanoparticle thin films have many functions in biosensing and microelectronics. The gold nanoparticle thin films are formed by self-assembly on silicon dioxide glass microscope slides through a layer-by-layer immersion technique. Gold nanoparticles (AuNPs) are employed to make these films because AuNPs have previously been shown to be biocompatible, relatively inert, and form monolayers rather easily. However, the temporal degradation of the thin films in an aqueous medium prevents their widespread use in biological applications. The degradation of the thin films is quantified by measuring the contact angle. Previously, it had been assumed that the decrease in contact angle, and thus the degradation, was due to desorption of the AuNPs from the film. However, analysis by ICP-OES after a moderate time period did not indicate loss of AuNPs from the films, and instead indicated a desorption of the outer layer of dodecanethiol from the slides.

05.05.38 Progress Towards the Synthesis of 1 α -Hydroxyvitamin D5 Core System

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This research project presentation describes the six-step synthesis of the core fragment of 1 α -hydroxyvitamin D5, a new, highly potent cancer chemopreventive agent, that was able to reduce the tumor incidence up to 47% and tumor multiplicity up to 50% in chemically-induced mammary carcinogenesis experiments in rats. This six-step synthesis project is part of a larger synthetic project aiming to develop an improved, convergent synthesis of the cancer chemopreventive agent 1 α -hydroxyvitamin D5, as a better alternative to the current 18-step linear synthetic approach. The starting material for this synthesis was vitamin D2 that was first converted into a sulfur dioxide adduct. The free hydroxyl group of the sulfur dioxide adduct was protected as a triethylsilyl ether, followed by selective cleavage of the vitamin D2 side chain via ozonolysis and reduction of the generated aldehyde to the corresponding alcohol, that represents the fourth intermediate in the synthesis of 1 α -hydroxyvitamin D5 core system. The alcohol will be further converted into a tosylate and the sulfur dioxide will be extruded from the adduct to yield the "trans"-vitamin D triene system, that constitutes the target molecule of this research project.

05.05.39 Regiospecific Lithium Mediated S_N2 Benzoylation of a Natural Anthoquinonoid Dye

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Research shows that disperse dyes containing additional –OR groups (R = methyl, alkyl or phenyl) have better sorption onto certain fabrics. Thus by tailoring the functionality of the hydroxyl groups it may be possible to synthesize natural dye derivatives with good compatibility to these fabrics. As the sorption of hydrophobic dyes onto biodegradable synthetic fabrics can be improved by substituting non-polar groups onto more polar functionalities, it is possible to develop simple and specific reactions to synthesize natural dye derivatives to replace artificial dyes. In this study we aimed to achieve efficient production of a mono di-ether Purpurin product. We produced a regiospecific reaction mixture with lithium acetate. The product from this reaction was extracted, dried, and concentrated in vacuo. The product was recrystallized in ethylacetate to afford a dark red solid and compared to the general reaction. TLC and ¹H NMR spectroscopy confirmed an ether linkage solely on the 2-position, creating a mono-product with a decreased polarity. Results support that our technique efficiently produces the preferred mono di-ether Purpurin product.

05.05.41 The Production of Xanthan Gum as a Sustainable Source of Hydraulic Fracturing

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For many years, scientists have been searching for more sustainable ways to support life on Earth. The fossil fuels that have been used for millions of years are depleting, leaving researchers to find quick solutions. Hydraulic Fracturing is a fairly new process that extracts natural resources from the shale layer of the Earth. How exactly do we get the resources without damaging and contaminating the environment? To date, Guar Gum and Kerosene are being used to produce fracking fluid that makes the process run smoothly. However, these two products are non-biodegradable and expensive. This project investigates how to efficiently produce a less expensive, biodegradable Xanthan Gum product. Xanthan Gum is derived from *Xanthomonas campestris* found in plants. *X. campestris* was planted on 3 different types of media to analyze the best method for growth; a solid, liquid, and intermediate media. Results demonstrated only immobilization of *X. campestris* allowed growth and enabled us to produce Xanthan Gum. Using our efficient technique to produce Xanthan Gum will be beneficial for two reasons. First, growing Xanthan Gum from Immobilized Bacteria would secure the food supply and reduce its cost; presently most of the fracking gum is taken from the food supply, adding to elevated food prices. Second, this technique may reduce America's gas prices and dependency on foreign oil by making fracking more sustainable via using less expensive techniques and using biodegradable material

05.05.42 Electrochemical redox mechanism analysis of $\text{Li}_{2-x}\text{FeP}_2\text{O}_7$ ($0 \leq x \leq 1$) pyrophosphate cathode via IR spectroscopy

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Northeastern State University

Effective materials for assembling electrochemical cells are an important and rapidly advancing focus in the industrial and scientific world. $\text{Li}_2\text{FeP}_2\text{O}_7$ has been structurally and electrochemically reported and confirmed, however more study on the redox mechanism is needed to advance the understanding of cathode performance. We are interested in the analysis of $\text{Li}_2\text{FeP}_2\text{O}_7$ via infrared spectroscopy to deduce and contribute to plausible redox mechanisms. Electrochemical extraction of lithium ions from the cathode material affects the electron distribution within the P-O bonds, and thereby affects the vibrational frequencies and IR band intensities. Thus, IR spectroscopy provides insight into the delithiation process from the perspective of the P_2O_7 anions. Before the analysis could be carried out, the cathode material had to be synthesized through a solid-state procedure and precursor mixture modeled by previous work. Once the material was synthesized, powder x-ray diffraction was performed to verify the desired product was prepared. The chemical delithiation of $\text{Li}_2\text{FeP}_2\text{O}_7$ was attempted with nitronium tetrafluoroborate in acetonitrile to produce cathode material that is free from conductive carbon and binder materials typically present in a battery cathode. Experimental data is presented demonstrating that the desired material has been obtained and the chemical oxidation may be an effective means to extract lithium ions from the compound to prepare a series of $\text{Li}_x\text{FeP}_2\text{O}_7$.