

DAYTON ACS ANNUAL POSTER SESSION
AND
PATTERSON COLLEGE CHEMISTRY AWARDS



APRIL 19, 2017

WRIGHT STATE UNIVERSITY

ENDEAVOUR ROOM

AGENDA

5:30 pm – 6:00 pm: Poster setup

6:00 pm – 7:30 pm: Poster session and judging

7:30 pm: Welcome address from the Dean of College of Science and Mathematics at Wright State University and award ceremony

2017 DAYTON SECTION OFFICERS

Chair: Dr. Eugeniya K. Iskrenova-Ekiert

Chair-Elect: Dr. Anastasie Weaver

Immediate Past Chair: Dr. Freddie Jordan

Secretary: Kerra Fletcher

Treasurer: Dr. Prakriti Basak Pollack

Councilor: Dr. Steve Trohalaki

Alternate Councilor: Dr. Rachel Jakubiak

1. TWO-DIMENSIONAL NANOPARTICLE ARRAY AND CLUSTER FORMATION BY SUPERCRITICAL FLUID DEPOSITION

Joanna S. Wang,¹ Gail J. Brown,¹ Chien M. Wai,² and Scott D. Apt¹

¹Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio 45433-7707, United States

²Department of Chemistry, University of Idaho, Renfrew Hall, Moscow, Idaho 83844, United States

Nanoparticles (NPs) can be deposited as two-dimensional (2D) clusters into nanostructures of silicon substrate using supercritical fluid CO₂ (sc-CO₂) as the medium. Due to its unique properties including gas-like penetration, liquid-like solvation and near zero surface tension, sc-CO₂ is capable of depositing NPs into nanometer-sized shallow wells which cannot be achieved by traditional solvent deposition methods. Nanoparticles tend to fill nano-structured shallow wells first, and then, if sufficient nanoparticles are available, they will continue to cover the flat areas nearby, unless defects or other surface imperfect areas are available. SEM images of two-dimensional gold (Au) nanoparticle arrays formed on silicon surface from 2 to a dozen or more of the Au nanoparticles are given to illustrate the patterns of nanoparticle array formation in sc-CO₂. Formation of large 2D NP arrays on silicon substrate surface is also described.

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2. MARCH FOR SCIENCE – DAYTON SATELLITE

Steve Trohalaki^a and Jessica Eby^b

- a) Sinclair Community College, Dayton, Ohio
- b) Eclectic Hat, Dayton, Ohio
steven.trohalaki@mac.com

The March for Science is a celebration of our passion for science and a call to support and safeguard the scientific community. Recent policy changes at the federal level have caused heightened concerns among scientists of every discipline. It has become increasingly clear that these concerns are shared by hundreds of thousands of people across the nation and around the world. The mischaracterization of science as a partisan issue, which has given policymakers permission to reject overwhelming scientific evidence, is an urgent matter and critical to the future of our country and humankind. It is high time for individuals who support scientific research and evidence-based policies to take a public stand and be counted.

ON APRIL 22, 2017, WE WALK OUT OF THE LAB AND INTO THE STREETS!

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3. Iron-bis(dithiolene) *N*-Heterocyclic carbene adducts as Pre-catalysts for Organocatalysis

Selvakumar Jayaraman and Kuppuswamy Arumugam*

Department of Chemistry, Wright State University, Dayton, Ohio.

e-mail: kuppuswamy.arumugam@wright.edu

The intriguing electronic and photophysical properties of transition metal dithiolene complexes continue to remain an active research area. Donahue et al demonstrated the reversible electrochemical release of triphenylphosphine from five coordinated Iron bis(dithiolene)-triphenylphosphine adducts. We envisioned a similar reversible release of *N*-heterocyclic carbene (NHC) with Iron bis(dithiolene)-NHC adducts would be possible under electrochemical conditions. Since, NHCs are ubiquitous in homogeneous catalysis, particularly in organocatalysis, a controlled reversible release is exceedingly attractive in this arena. Herein, an electrogenerated NHC catalyzed cyclo-trimerization of phenylisocyanate and synthesis of γ -butyrolactone from cinnamaldehyde is discussed.

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4. MEASURING THE BINDING ENERGY OF GLUCOSE TO THE GLUCOSE/GALACTOSE BINDING PROTEIN COMPUTATIONALLY

Nicholas R. Rigel '18* and Dr. A. G. Anderson

Department of Chemistry | Wittenberg University | Springfield, OH

The Glucose/Galactose Binding Protein (GGBP) is crucial to bacterial chemotaxis in *E. coli* and other bacteria, binding either to glucose or galactose¹. GGBP is an α/β protein consisting of two globular Rossmann fold domains joined by three peptide segments^{2,3}. Since GGBP binds to glucose in *E. coli*, it has the possible use as a bio-indicator in diabetes patients⁴. GGBP normally exists in its closed conformation (*Figure 1A*) and opens to bind to glucose (*Figure 1B*)⁵. GGBP binds to glucose with a hinge feature that causes the protein to close around the sugar. A hinge angle exists between a residue in each domain and a residue near the binding pocket. A molecular dynamics method of umbrella sampling was implemented to not only show the conformation change when GGBP binds to glucose, but also measure the Gibb's free energy of binding. An angle change of 23.5° was observed experimentally, while 22.0° was observed from umbrella sampling¹. The experimental Gibb's free energy of binding of GGBP to glucose is -9.1 kcal/mol, while a binding energy of $-10.4(\pm 0.4)$ kcal/mol was measured by umbrella sampling⁶.

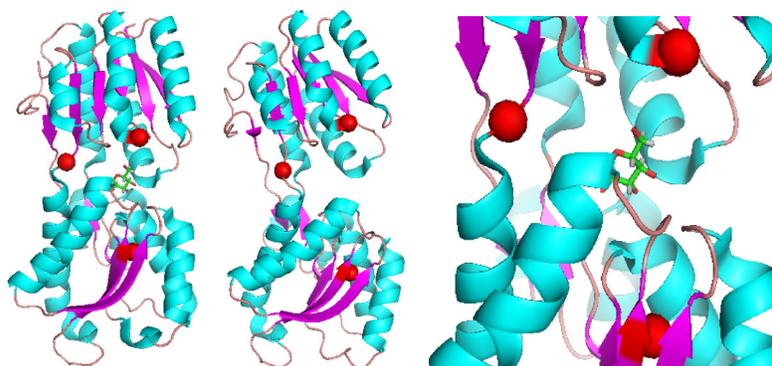


Figure 1. (A) shows GGBP with bound glucose and (B) shows GGBP without glucose, from RCSB files 2fvy and 2fw0, respectively¹. (C) is the binding site, red spheres are the residues used in angle analysis.

*Undergraduate

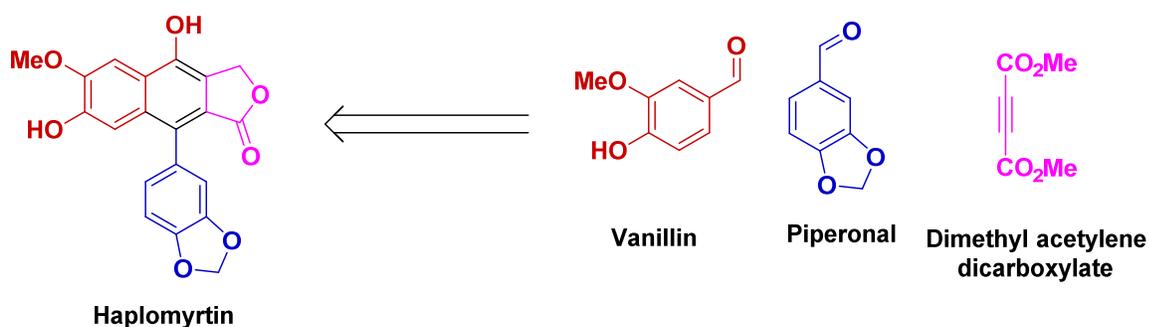
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5. IMPROVEMENTS TO THE SYNTHESIS OF HAPLOMYRTIN AND SYNTHESIS OF A TRIFLUOROMETHOXY ANALOGUE

James Herbort^a and Willaim A. Feld^a

c) Wright State University
Jamesherbort@gmail.com

Aryl naphthalene natural products have been shown to inhibit HT-29 colon cancer cells in mammals by a method that is dissimilar to the commercially available cancer drug Etoposide. Haplomyrtin bears a striking resemblance to many biologically active aryl naphthalene molecules, but it's potency (or lack thereof) remains untested. A seven-step strategy led to the synthesis of haplomyrtin in a 7% overall yield. The installation of the pendant moiety allows for easy access to different analogues. To evidence this, studies are being done to synthesize an analogue which contains the very lipophilic trifluoromethoxy group.



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6. GOLD (I) COMPLEXES CONTAINING ALKYLATED FERROCENES: THE BEGINNING OF A NEW GENERATION OF ORGANOMETALLIC ANTI-CANCER COMPOUNDS

Don Hoang; Selvakumar Jayaraman; Dr. Kuppuswamy Arumugam

Wright State University Department of Chemistry

Implementing redox-active organometallic compounds can increase intracellular reactive oxygen species (ROS) levels, leading to oxidative stress and eventually apoptosis in neoplastic cells. It is hypothesized that reducing the redox potential of the compound would facilitate redox processes, increasing the overall potency of the compound. Accordingly, the goal of the project is to synthesize imidazolinium salts that could allow for tuning of redox potential in ferrocenyl-N-heterocyclic carbene gold (I) complexes. Carbamoyl ferrocene seemed to provide the best route to the desired imidazolinium salts. The next steps are lithiation of carbamoyl ferrocene followed by electrophilic substitution and Friedel-Crafts acylation of carbamoyl ferrocene. Once the imidazolinium salts are prepared, they will be subjected to preparation of gold (I)-N-heterocyclic carbenes.

**Undergraduate; Competing for an Award

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7. SOURCE DETERMINATION OF ARSENIC, LEAD, AND CADMIUM IN THE YELLOW SPRING SEDIMENT IN GLEN HELEN NATURE PRESERVE, OH

Warren, Emily L., McGowin, Audrey E., Teed, Rebecca E., Sanders, Scott

Arsenic, lead, and cadmium have been found at elevated levels in the sediment of the “Yellow Spring” located in Glen Helen Nature Preserve in Yellow Springs, Ohio (A. McGowin, unpublished results). The Yellow Spring is named for the bright orange travertine deposits that are rich in iron. My research was to determine whether the arsenic, lead, and cadmium in the sediment were occurring naturally in the spring or coming from the pipes that are used in the construction of the man-made structure from which the artesian spring flows. I collected sediment samples from three surrounding sights for comparison. The first three sample sites were the Yellow Spring sediment, the “Grotto” sediment (a waterfall just downstream), and a second site further downstream site. Another site was soil from the root zone of a fallen tree that is also rich in iron, from which three samples were taken. A total of six samples, each sample split into four replicates for analysis. Samples were digested in acid following USEPA Method 3050B and analyzed for iron, arsenic, lead, and cadmium using inductively-coupled plasma-optical emission spectrometry (ICP-OES) following EPA Method 200.7. Statistical analysis of the results indicate that arsenic, lead, and cadmium occur naturally in minerals that are distributed throughout Glen Helen.

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8. Development of Synthesis Strategy for [Bis-(1,3-diferrocenylmethyl-imidazole-2-ylidene)-gold] [tetrafluoroborate]₅

Catherine Evers Smith¹ and Kuppuswamy Arumugam¹

¹Wright State University, ¹Department of Chemistry, Dayton, OH 45435-0001

**Corresponding author email: kuppuswamy.arumugam@wright.edu*

The group previously synthesized [Bis(1,3-diferrocenylmethyl-imidazol-2-ylidene)-gold(II)] [chloride]. This compound was observed to kill cancer cells in the body through dual mechanistic pathways, i.e., suppression of anti-oxidative enzyme and non-specific generation of reaction oxygen species. Ferrocene is believed to be involved in catalytic generation of reactive oxygen species. This aim of this project include isolation of oxidized version of [bis(1,3-diferrocenylmethyl-imidazol-2-ylidene)-gold] [tetrafluoroborate] to prove that oxidation occurs at ferrocene center. Therefore, a strategy for the synthesis of [bis(1,3-diferrocenylmethyl-imidazol-2-ylidene)-gold(II)] [tetrafluoroborate]₅ was developed.

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9. Characterization of $Cd_{1-x}Zn_xTe$ (CZT) Crystals for Radiation Detection

Daniel Lee^{a, b}*, Dr. Arnold Burger^a, Michael Groza^a, Vladimir Buliga^a, Dr. Yunlong Cui^a

^a *Fisk University, Physics Department, Nashville, TN 37208 USA*

^b *Central State University, College of Science and Engineering, Wilberforce, OH 45384 USA*

*Corresponding Author Email: dlee23@central.ces.edu

Keywords

($Cd_{1-x}Zn_xTe$ CZT), Zn distribution, Pockels electro-optic effect, detection response

Abstract

Commercial grade Cadmium Zinc Telluride ($Cd_{1-x}Zn_xTe$ CZT) crystals can be used as a radiation detecting medium for homeland and national security applications, medical imaging, and high energy astrophysics applications. CZT has a band gap between 1.4-1.7 eV, which is larger than that of Ge and Si, making it useful for variable temperature applications. CZT, unlike Ge and Si, detects gamma radiation efficiently at room temperature in normal atmospheric conditions. Its high Z number also makes it an excellent candidate for gamma radiation detection. We characterized two $Cd_{1-x}Zn_xTe$ (CZT) crystals grown at Washington State University (WSU), CG50 and CG83, through a series of physical tests. To determine important intrinsic characteristics of the CZT crystals, the various tests we performed include: near infrared (IR) transmission imaging, Zn distribution using Photoluminescence (PL) Mapping, Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), internal electric field uniformity testing utilizing the Pockels electro-optic effect, resistivity testing using current-voltage measurements, and lastly detection response testing. The findings of our research are reported back to WSU and other institutions for improving their CZT growing methodologies; which enables them to develop a more consistent high yield process for commercial grade CZT detectors.

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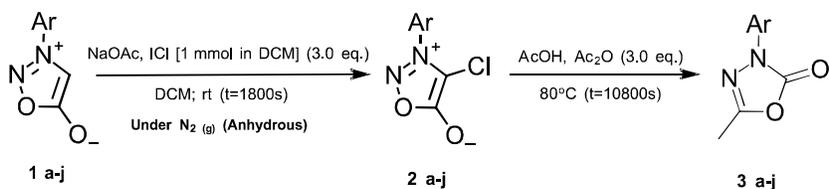
10. Chlorination of 3-Arylsydnes with Iodine Monochloride

Benjamin L. Owens^a, Jonathan M. Tumey^a, Imad F. Nashashibi, and Kenneth Turnbull*

a. Department of Chemistry, Wright State University, Dayton, OH 45435-0001

Sydnes are unique, dipolar heterocycles, which are members of the class of compounds known as mesoionic. The process of electrophilic aromatic substitution is an integral part of sydnes research and when the sydnes ring is unsubstituted at the 4-position it becomes very susceptible to electrophilic attack, which allows for a variety of different substitutions. The most common of these is halogenation and, while bromination has been the most studied, several methods have been developed for chlorination at the sydnes 4-position. Most of these, however, have considerable drawbacks including competing reactions, low yields, and/or the handling of harmful gases. Thus it was investigated as to whether an improved method of chlorination could be derived with the use of iodine monochloride (ICl). It was discovered that chlorination of the sydnes 4-position with ICl in DCM occurred under mild conditions, providing high product yields and purity, and short reaction times. In collaboration, the products synthesized *via* this procedure were then transformed into the corresponding 1,3,4-oxadiazol-2(3*H*)-ones by treatment with acetic acid in the presence of a limited amount of acetic anhydride. Thus, a novel approach to the synthesis of 1,3,4-oxadiazol-2(3*H*)-ones **3a-j** from 4-chlorinated-3-arylsydnes **2a-j** has been developed (Scheme 1). The scope and limitations will be presented.

Scheme 1: Synthesis of 4-chloro-3-arylsydnes from 3-arylsydnes and ICl followed by conversion of the latter to 1,3,4-oxadiazol-2(3*H*)-ones by treatment with acetic anhydride in acetic acid.



a, Ar = H; b, Ar = p-Cl; c, Ar = p-Br; d, Ar = p-CH₃; e, Ar = p-COCH₃;
 f, p-OCH₃; g, m-OCH₃; h, 3,4-DiCH₃; i, 2,3-DiCH₃; j, 2,4-DiCH₃;

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11. Resolving the Molecular Mechanisms by Which DNA Mutations Alter the Function of a Genetic Switch

Emily E. Wey¹ and Thomas M. Williams²

¹ Department of Chemistry, ² Department of Biology, University of Dayton, 300 College Park, Dayton, OH 45469

Each human genome possesses around a million mutations that are genetic baggage from DNA replication mistakes or “mutations” that occurred in the past. Each mutation can have one of three outcomes on an individual, these are to improve, reduce, or have no effect on health. Moreover, the effects of such mutations can depend on the presence or absence of other mutations, so called epistatic interactions. A major goal of genomic medicine is to glean diagnostic or predictive health information from the genome sequences of individuals. However, this goal remains out of reach as the effects of mutations and epistatic interactions are difficult to predict without knowing the function of the DNA sequence they reside in. This difficulty is especially heightened for mutations occurring in cis-regulatory element sequences that act as switches to control gene transcription. The research I am performing for my Honors Thesis, under the advisement of Dr. Thomas Williams, is to use a fruit fly model to test hypotheses about the molecular mechanisms by which mutations alter a genetic switch’s activity and whether these mutations are subjected to the tyranny of epistatic interactions. I will study the *Drosophila melanogaster* dimorphic element which is a transcription-regulating switch for the *bric-à-brac* genes. Three mutations in the dimorphic element were identified that individually alter the level of *bric-à-brac* transcription. The presence or absence of epistatic interactions will be determined by measuring the activity of dimorphic elements from related species that have been engineered to possess the *Drosophila melanogaster* mutations. I will also test the hypothesis that these mutations impart their effects by creating or destroying binding sites for proteins known as transcription factors. The results will provide a sorely needed example where an understanding of molecular mechanisms bridges the gap between a DNA sequence and its *in vivo* function.

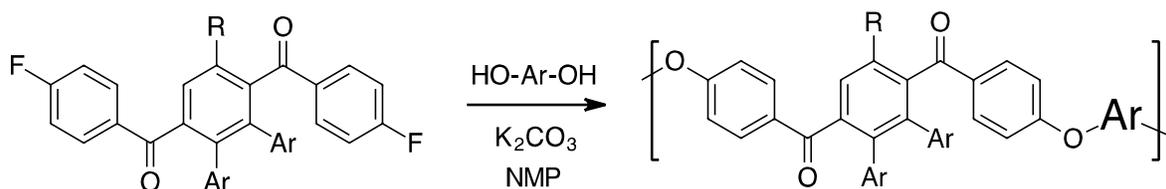
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12. SYNTHESIS OF ALKYL SUBSTITUTED PHENYLATED POLY(ETHER ETHER KETONE)S

Matthew Cerone^a and William Feld^a

d) Department of Chemistry, Wright State University, Dayton, OH 45435-0001
cerone.2@wright.edu

Poly(ether ether ketone)s are a much studied polymer family, best suited for use in industries where a resilient, nonreactive material is needed. One issue with PEEK is that it is difficult to process. The rigid structure, functional group polarity and planar aromatic character appear to be responsible. Adding pendent functionality, particularly phenyls, is known to increase solubility and processability. The NAS polymerization of bis(fluorophenyl) monomers **1a** and **1b** to the corresponding polymers **2a** and **2b** has been reported and the influence of the additional phenyl substituents documented. The addition of an alkyl chain in monomer **1c** led to polymers **2c** that exhibited a decrease in T_g with a minimal influence on thermal stability ($T_{d5\%}$). Polymers **2b** and **2c** were soluble in chloroform and were able to be cast as thin transparent films. A comparison of the properties of polymers **2a-c** will be presented.



1a Ar = H, R = H

1b Ar = -Ph, R = H

1c Ar = -Ph, R = -C₆H₁₃

2a Ar = H, R = H

2b Ar = -Ph, R = H

2c Ar = -Ph, R = -C₆H₁₃

**Graduate Student competing for award

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13. HYDROTHERMAL ATOMIC FORCE MICROSCOPY INVESTIGATION OF BARITE GROWTH: THE ROLE OF SPECTATOR IONS IN ELEMENTARY STEP EDGE GROWTH KINETICS AND HILLOCK MORPHOLOGY

Sarah A. Jindra, Angela L. Bertagni and Steven R. Higgins*

Department of Chemistry, Wright State University, Dayton, OH 45435-0001

[*steven.higgins@wright.edu](mailto:steven.higgins@wright.edu) (corresponding author)

Mineralization of barite (BaSO_4) occurs in various geologic settings where barite scale formation can be problematic. To better understand the role of spectator ions in the aqueous solution growth of barite, the kinetics of elementary step edge growth on barite (001) surfaces have been studied under a wide variety of solution conditions. The results of these studies have been used to determine the effects of various electrolytes on elementary step kinetics. Hydrothermal Atomic Force Microscopy (HAFM) was used to investigate the effect of background electrolytes (NaCl, NaBr and NaNO_3) as a function of saturation index, and ionic strength (I) on barite growth sourced at dislocations at 108 °C. Initial results show that hillock morphology is affected by I . The effect of increasing I on hillock morphology was observed in 0.05 M NaCl, but the effect was absent in 0.05 M NaNO_3 , suggesting a specific interaction of Cl^- with the polar [010] step edge in contrast to NO_3^- . The step rate coefficient increased when I was increased in NaCl solutions. Initial results for NaNO_3 further indicate an ionic strength effect on rate coefficients, however, the coefficients for NaCl tended to be larger than the NaNO_3 coefficient, possibly indicating an inhibitory role of nitrate towards the advancement of the non-polar $\langle 120 \rangle$ steps. These results indicate that I is a driver of hillock morphology in the instances where NaCl is the electrolyte. However, in the case of NaNO_3 there is no clear driver for the morphology.

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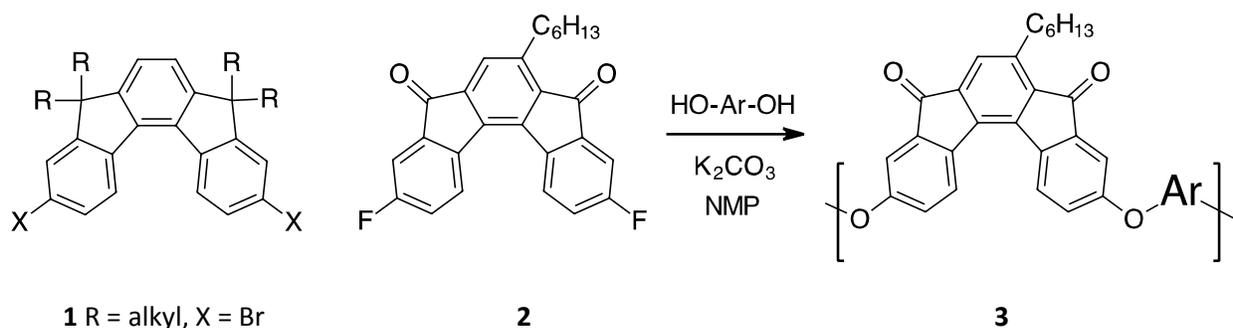
14. INCORPORATION OF 5,8-DIOXO-5,8-DIHYDROINDENO-[2,1-C]FLUORENE INTO POLYMERIC SYSTEMS

Nathaniel T Brackett.¹ William A. Feld²

¹Department of Chemistry, Wright State University, Dayton, OH 45435-0001

*brackett.3@wright.edu

Indenofluorenes **1** show many desirable properties crucial to today's modern technologies. They have excellent emission and absorption wavelengths which make them ideal for organic light emitting diodes or organic photovoltaic devices. They are usually incorporated into polymers by coupling reactions using either nickel or palladium catalysts. As a complement to those methods, a five-step synthesis resulted in the formation of 3,10-difluoro-5,8-Dioxo-5,8-dihydroindeno-[2,1-*c*]fluorene **2** that could undergo polymerization by nucleophilic aromatic substitution. Monomer **2** was reacted with *p*-cresol in a model reaction and with bisphenol-A to produce polymer **3**. A discussion of the multiple reaction conditions employing NMP and DMSO in these reactions will be presented.



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15. LIGHT INDUCED COLOR CHANGES IN THE PURPLE PROTEIN BACTERIORHODOPSIN

Carlie McGrath^a, Mark Masthay^b, and Angela Mammana^b

a) University of Dayton, Department of Chemistry, Dayton, Ohio 45409, USA

This research provides new insights into the mechanisms associated with light-induced color changes in the bacteriorhodopsin (BR)-containing halobacterial purple membrane (PM). BR is a purple, 26kDa transmembrane protein which is structurally similar to the human visual proteins rhodopsin and iodopsin.

This research focuses on the influences of light scattering and spectral distortions induced by the solvent in which PM is suspended. Various volume ratios of water and glycerol were used as the solvent for PM samples. A ratio of 60% glycerol:40% water produced spectra with the least scattering, as demonstrated by a low absorbance region (300-420 nm) in the UV-visible absorption spectra and equal intensities of the positive and negative bands in the circular dichroism (CD) spectra. Suspensions of native PM, calcium saturated purple membrane (CSPM) and cation free blue membrane (CFBM) were irradiated with intense 532 nanometer (nm) laser pulses. During irradiation the absorption and CD spectra were monitored.

PM and CSPM each produced a UV product with λ_{max} ~360 nm, while no peak was observed in CFBM. Upon laser irradiation, the absorption spectra of both PM and CSPM “crossed over” (*i.e.*, the long wavelength edge of the main absorption band shifted bathochromically) during the early stages of irradiation; this “crossing over” was absent in CFBM. PM also underwent a later bathochromic shift of its absorption λ_{max} with a concomitant purple-to-blue color change. Both CSPM and CFBM underwent a color loss but no color change. Implications of these findings are detailed below.

**I am a graduate student and would like this poster to be considered for judging.

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16. HEAVY METALS IN LYTLE CREEK AND INDIAN RUN

Amira M. Alsenbel and Audrey E. McGowin*

¹Department of Chemistry, Wright State University, Dayton, OH 45435-0001

Taylor Stuckert, Clinton County Regional Planning Commission, Wilmington, OH

Lori Williams, City of Wilmington, Parks and Recreation Director

Harry McVey, City of Wilmington, Wastewater Superintendent

alsenbel.2@wright.edu, *audrey.mcgowin@wright.edu

Limited macroinvertebrate biodiversity in Lytle Creek that runs through downtown Wilmington, OH has been documented over decades with the lowest in Lytle Creek at Sugar Grove Cemetery. Lytle Creek, a tributary of the Little Miami River, is a conduit for storm water and wastewater from an airport, downtown storm water with input from local businesses, and a wastewater treatment plant. This study was conducted to see if heavy metal pollution in the sediment could be a contributing factor in reduced macroinvertebrate populations. Five sites were sampled in Lytle Creek from the headwaters at Wilmington College to the landfill discharge. A tributary to Lytle Creek, which runs through downtown at Xidas Park, was added when dead fish were discovered. Two sites were selected in Indian Run, one upstream and one downstream of the airport's wastewater treatment facility. Sediments were analyzed for mercury (Hg) using cold vapor atomic fluorescence spectrometry. Aluminum (Al), arsenic (As), cadmium (Cd), chromium (Cr), copper (Cu), iron (Fe), manganese (Mn), nickel (Ni), lead (Pb), strontium (Sr), and zinc (Zn) were determined by inductively-coupled optical emission spectrometry (EPA method 200.7). Mercury concentrations ranged from 0.013-0.163 mg/kg dry wt. The highest levels of mercury were found in Xidas Park and in Sugar Grove Cemetery (0.124 and 0.163 mg/kg dry wt., respectively). Total heavy metals ranged from 0.014-340 mg/kg dry wt. The downtown tributary to Lytle Creek, Xidas Park site, empties into Lytle Creek at Sugar Grove Cemetery indicating lack of biodiversity in Lytle Creek may be caused by runoff into storm drains in downtown Wilmington.

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17. DEVELOPMENT OF N-HETEROCYCLIC CARBENE-GOLD(I) COMPLEXES FOR THERAPEUTIC APPLICATIONS

Meredith Miles,^a Rebecca McCall,^b Jannet Kocerha,^b Kevin Sidoran,^c Jonathan F. Arambula,^{b,d}
Kuppuswamy Arumugam,^{a,*}

^a Department of Chemistry, Wright State University, Dayton, OH 45435, USA

^b Department of Chemistry, Georgia Southern University, Statesboro, GA 30460, USA

^c Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY 14778, USA

^d Department of Chemistry, University of Texas, Austin, TX 78712-1224, USA

The tunable steric and electronic properties of N-heterocyclic carbenes (NHCs) coupled with their σ -donating abilities allow for excellent coordination to transition metal complexes. NHC-gold(I) complexes have shown promise as cancer treatment drugs because of their ability to target thiol-functional groups found in the Thioredoxin Reductase (TrxR) system. Our previous work has proven that generating reactive oxygen species (ROS) and inhibiting the TrxR system simultaneously induces apoptosis. Hence, modifying the N-substituents and fusing the NHC-gold(I) complex with naphthoquinone further enhanced this oxidative-stress pathway to kill the tumor cells. Three naphthoquinone fused NHC-gold(I) complexes were synthesized and confirmed structurally with ^1H and ^{13}C NMR, UV-Vis spectroscopy, IR spectroscopy, and X-ray crystallography. The redox properties of the complexes were confirmed with various electrochemical techniques. Cell proliferation studies were also performed to determine the efficacy of the complexes.

**Graduate student at Wright State University competing for student awards.

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18. EFFECTS OF CROSS-LINK DENSITY AND SPACING ON THE PROPERTIES OF HIGH TEMPERATURE SULFONAMIDE-BASED ELASTOMERS

Shannon Hennelly Wright State University, Eric Fossum* Wright State University

Elastomers have applications in the automotive, construction, energy and manufacturing industry. Elastomers consist of polymer chains that are crosslinked together and they tend to have low glass transition temperatures, T_g 's, and a low shear modulus. In this research poly(arylene ether)s, PAE's, based on *N,N*-dialkylbenzene sulfonamides, were employed because of their good thermal properties. All of the monomers are designed for conversion to polymeric form using standard nucleophilic aromatic substitution, NAS, polycondensation reactions. The length of the alkyl chains provides the opportunity to tailor the glass transition temperature, T_g , of the final material. Sites for crosslinking can be incorporated with diallyl monomers and various cross-link densities can be achieved. By utilizing monomers with different levels of reactivity toward NAS reactions, it should be possible to piece the components together using a modular approach, thus controlling the placement and number of crosslinks. The resulting polymers will be fully characterized and then crosslinked to form the desired elastomers, at which point their shear moduli will be determined and thorough structure-property relationships will be developed. The initial data will then be used as a guide for development of the next generation of high temperature elastomers.

ACKNOWLEDGEMENTS: Wright State University College of Math and Science, Wright State University Chemistry Department

19. Structure-Property Relationships of Polymerizable Blue-Emitting, π -Donor: π -Acceptor Chromophores for OLED Applications

Amy McNeely Wright State University, Eric Fossum Wright State University

An organic light emitting diode (OLED) is a self-emitter that does not require the use of rare earth metals, as is the case with inorganic light emitting diodes (LEDs). Currently, red and green emitters have achieved longer lifetimes and efficiency than blue emitters. In order to enhance the long-term stability our approach utilizes a benzoxazole core to which can be added a variety of donors. The choice of benzoxazole is based, in part, on its successful application in a number of thermally and oxidatively stable polymeric systems. The approach provides a unique opportunity to tune the band gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), and, in turn, the emission wavelength, without substantially altering the core structure. The chromophores are designed to undergo efficient thermally activated delayed fluorescence (TADF), which allows harvesting of both the singlet, via fluorescence, and triplet states, by fluorescence after reverse intersystem crossing (RISC). In addition, the modular approach also provides an avenue to covalently incorporate the chromophores into polymeric systems via nucleophilic aromatic substitution (NAS). As such, our initial chromophores were chosen with 2,4-difluorinated rings, attached at the 2-position of the benzoxazole system, which are capable of undergoing NAS polycondensation reactions. This presentation will focus on the synthesis, characterization, and polymerization behavior of benzoxazole-based, blue emitting chromophores.

ACKNOWLEDGEMENTS: Wright State College of Science and Math, Wright State Chemistry Department

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20. Cloud Point Extraction (CPE) in combination with Tangential Flow Filtration (TFF) for the isolation of silver nanoparticles and ionic silver

Md Ali Akbar¹, Sessa Paluri^{1,2}, Ioana Sizemore^{1,2*}

¹Department of Chemistry, ²Biomedical Sciences Ph.D. Program,
Wright State University, Dayton, Ohio, 45324
akbar.7@wright.edu

The increased use of silver nanoparticles (AgNPs) in a variety of consumer products has amplified their potential release into the environment. Furthermore, AgNPs were found to exert harmful effects on living organisms mostly by producing Ag⁺ ions and causing oxidative stress. Therefore, it is imperative to develop methods for isolating the two silver species (AgNPs and Ag⁺) from various matrices. In this study, cloud point extraction (CPE) and tangential flow filtration (TFF) were combined to increase the extraction efficiencies of AgNPs and Ag⁺ from colloidal and biological matrices. Briefly, a non-ionic surfactant (Triton X-114) and sodium thiosulfate were added to the samples containing AgNPs and incubated over the cloud point temperature of the surfactant to allow for the micelle formation with AgNPs (surfactant phase) and the chelation of Ag⁺ with thiosulfate (aqueous phase). The two CPE phases were then separated by centrifugation, and the aqueous phase containing mainly Ag⁺ ions and some AgNPs was further processed through a 1-kD filter to further recover AgNPs. The total concentration of Ag in the two CPE phases and the resulting TFF products, namely permeate (containing Ag⁺) and retentate (containing AgNPs), were quantified by inductively coupled plasma optical emission spectroscopy (ICP-OES). The versatility of the CPE-TFF method was demonstrated on three different colloids (Creighton, Citrate-capped, PVP-capped) and one cellular matrix (animal kidney cells). The extraction efficiency of AgNPs and Ag⁺ ranged from ~65%-88% and 15-28% respectively, while the total Ag recoveries were from 81% to 96.43%.

(G)

21. A Stochastic Cellular Automaton Model of Tautomer Equilibria

Gregory Bowers^a and Paul Seybold^{a*}

a) Department of Chemistry, Wright State University, Dayton, OH 45435

Tautomer equilibria are complex and dynamic, making modeling them a challenge. Cellular automata models are uniquely suited to address this challenge, allowing the equilibria to arise naturally from simple rules. In this study, a stochastic, asynchronous cellular automata model was employed to simulate the tautomer equilibrium of 9-anthrone and 9-anthrol in the presence of their common anion. The observed K_E of the 9-anthrone \rightleftharpoons 9-anthrol tautomerization along with the measured tautomer pK_a values were used to model the equilibrium at pH values 4, 7, and 10. At pH values 4 and 7, the anthrone comprised >99% of the total species population, whereas at pH 10 the anthrone and the anion each represented just under half of the total population. The anthrol population was very small under all conditions.

(G)

22. Adsorption of Fullerenes on Alumina: A Molecular Simulation Study

Richard A. Williams^a and Rachel S. Aga^a

e) Department of Chemistry, Wright State University, Dayton, OH 45435-0001

From drug delivery to solar cells, fullerene molecules and their derivatives are being utilized for applications in a variety of technologies. They are poised to become increasingly important in the future of science and engineering. With the increased use of these molecules, it is important to investigate how they will interact with other natural materials to understand their potential impact on the environment. We explore the adsorption behavior of C60 and C70 molecules on alumina, a common mineral in the environment, through the use of molecular simulations. With this technique, we aim to provide a molecular-level understanding of the properties at the nanomaterial-mineral interface. Simulations consisting of a series of geometry optimizations and molecular dynamics were carried out using Materials Studio. We report density profiles and adsorption energies as a function of nanomaterial concentration. The trend in the adsorption energy is consistent with the local ordering of the fullerenes at the interface. It was observed that clustering appears to be favorable for both molecules, as the adsorption energy decreased with increasing density. Simulations with water were also carried out, and we find that the density distributions of the fullerenes near the mineral surface are altered by the presence of water.

(G)

23. Redox-active Silver N-Heterocyclic Carbene Complexes: A Dual Targeting Anti-bacterial Drug

Kotiba Malek, Krushangi Shah, Alexander Castillo Guel and Dr. Kuppaswamy Arumugam*

Malek.5@wright.edu

Bacterial resistance to current antibiotics necessitates new alternative therapeutic drugs. Silver based drugs are promising in this realm. However, current silver-based antibacterial drugs are limited in their bioavailability due to their rapid release of silver ions. Recently, *N*-heterocyclic carbene containing silver complexes have gained popularity due to slow release of silver ions under biological conditions. As a result, two new potential antibacterial silver-NHC complexes were synthesized and confirmed via analytical techniques, including ^1H and ^{13}C NMR spectroscopy and x-ray crystallography.

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PATTERSON COLLEGE CHEMISTRY AWARDS

The Patterson College Chemistry awards are administered by the Dayton Section of the American Chemical Society and are presented annually to outstanding junior chemistry majors at each college and university within the Section's boundaries. The recipients of the Patterson College Chemistry Awards are chosen by the faculty of each college or university from their outstanding juniors using the general criteria of scholarship, character, extra-curriculum involvement, and potential for success after college.

This year, the awardees are:

- Cody Fourman Wright State University
- Dexter Heath Central State University
- Jessica Skoglund Wittenberg University
- Emily Wey University of Dayton

The following pages contain short biographical sketches of the honorees. The Dayton Section offers its most sincere congratulations to these distinguished students.

PATTERSON COLLEGE CHEMISTRY AWARDS

Jessica Skoglund

Wittenberg University

Introduced by: Prof. Justin Houseknecht

Jessica Skoglund is a Junior Chemistry and Mathematics double major at Wittenberg University. This summer she conducted research at her undergraduate with her chemistry advisor, Dr. Ray Dudek. Her research included learning a higher level statistical test, Principal Component Analysis, in order to differentiate authentic and adulterated Extra Virgin Olive Oils based on their infrared spectra. She continued research into the fall semester of her junior year, this time looking at methods to create, tarnish, and then polish silver nanoparticles monitored by UV-Visible spectroscopy.

Outside of research, Jessica is the Vice President of Wittenberg's Chemistry Club where she helps plan a Wittenberg Science Night with the local Girl Scout Troops who are invited to come and learn about various STEM activities and opportunities. She holds a job on Wittenberg's campus as a general chemistry laboratory teaching assistant. She has served as an executive officer of her sorority for the past two years and is the President of Omicron Delta Kappa, an academic and service-based Greek honorary.

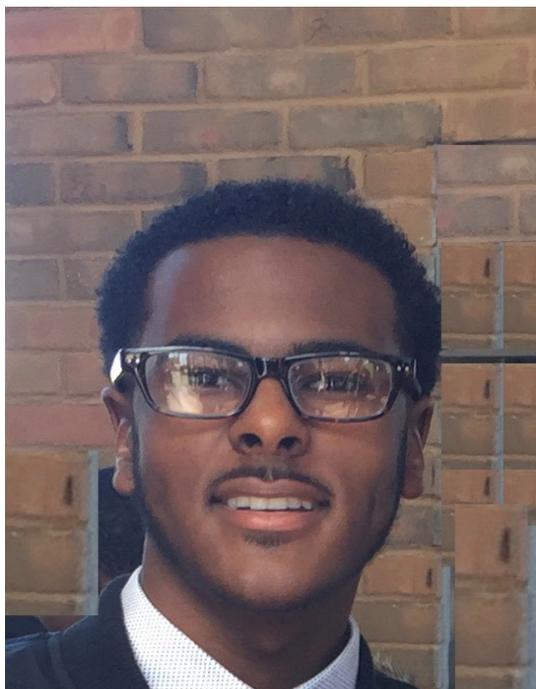
In her free time, she enjoys being outside and you will often find her under two trees in her hammock. She regularly attends Trivia Nights hosted by her advisor, on campus comedy shows, and serves her community through various campus sponsored projects such as service immersion trips (which she attended this past spring break). She is from Westerville, Ohio and loves to go home when she can to visit her dog, Oreo. She aspires to be a pediatrician and is currently studying for the MCAT that she will be taking in May. She is thoroughly enjoying her time at Wittenberg and is excited to see where her future takes her.

PATTERSON COLLEGE CHEMISTRY AWARDS

Dexter Heath

Central State University

Introduced by: Prof. Leanne Petry



Dexter Heath was born on November 3rd, 1996 to Debra and Derek Heath. He was raised in Prince George's County Maryland, a suburb 20 minutes from the nation's capital. He is currently pursuing a Bachelor of Science degree in Chemistry at Central State University.

Dexter is involved with many activities on campus. He is an Ag-STEM Institute Scholar (USDA), the Executive Secretary for the Student Government Association (SGA), a member of Family Community Leadership in Action (FCLA), and a model for Iconic Models. Dexter prides himself on doing whatever it takes to help improve his current school for future students to receive the same great HBCU experience as he did. Dexter has dedicated himself to being a scholar, is part of the Honors Program, and is a resident advisor at Central State University.

Last summer 2016, Dexter participated in a 10-week internship program at Case Western Reserve University with the Department of Macromolecular Science and Engineering. Dexter's research at Case focused on the effectiveness that Lignin and Polyvinylamine had on removing toxic metals from water tainted with lead. In the future, Dexter plans to pursue a graduate degree in forensic pathology.

PATTERSON COLLEGE CHEMISTRY AWARDS

Emily Wey

University of Dayton

Introduced by Prof. Thomas Williams

Emily Wey is from Mason, Ohio and is currently a junior Biochemistry major on the Pre-Med track at the University of Dayton (UD). Emily's undergraduate research is the study of whether function altering mutations are susceptible to epistatically relating sequences using *Drosophila melanogaster* as a model organism. She is developing this research into an Honors Thesis with Dr. Thomas Williams as her thesis advisor. Emily was a member of the 2016 Berry Summer Thesis Institute cohort at UD which allowed her to get a strong start on her thesis project. In addition to her undergraduate research, Emily is Vice President of Beta Beta Beta (Biology Honor Society) and she is actively engaged in Alpha Epsilon Delta (Premedical Honor Society) and Optimist International Club (Service club). Emily is an active volunteer in the Dayton community. The two service projects she has been most involved with are her long-term volunteer position in the Day Surgery department at Dayton Children's Hospital as well as her medical scribing role and triage role with Reach Out of Montgomery County (free clinic for underserved population). After graduation, Emily plans to attend medical school to pursue a career in medicine.

PATTERSON COLLEGE CHEMISTRY AWARDS

Cody Fourman

Wright State University

Introduced by Prof. Audrey McGowin

Cody Fourman is a first-generation college student from his family's farm in Arcanum, Ohio, where he is majoring in Chemistry and minoring in Music. Cody graduated from Arcanum High School, where his high school chemistry teacher was inspiration to pursue a higher education in chemistry. He is currently working on a research project at Wright State with Dr. Ketcha exploring anticancer compounds. Cody also works as an associate research assistant at the Wright-Patterson Air Force Base. If that weren't enough, he is a valuable student instrument specialist for the Wright State chemistry department, helping to keep all the instruments running. Cody's plans after graduating remain open-ended, but he hopes to put his chemistry degree to good use, and to continue learning in the field of science. Hopefully, he will still find time to play the saxophone.