

Received: 2/26/2013

Abstract 1P (1st professional, non-award)

Stability Studies of PbS Colloidal QD Films on Glass and GaAs Substrates

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Lead Sulfide (PbS) quantum dots (QDs) have attracted considerable attention due to their ability to provide large quantum confinement energies, which paved the road for novel technological applications. Although there are myriad studies involving PbS deposition, hardly any have demonstrated the stability of PbS QD films on GaAs substrates. In this analysis, PbS QD film deposition on semi-insulating GaAs was compared to that on glass substrates using a supercritical fluid CO₂ (scCO₂) deposition method (SFD) and a solvent deposition method (SDM). Over a period of months, the QD film samples were re-tested after being left unprotected in air under ambient conditions. We also tested the samples which remained at ambient conditions for over 2 years. Despite exposure to laser excitation at 532 nm and cooling to cryogenic temperatures, the photoluminescence (PL) initially remained stable between tests. To track potential changes to the QDs over time, PL, X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), X-ray diffraction (XRD), optical microscopy, and atomic force microscopy (AFM) studies were employed. Our stability standard protocols are important for reliability expectations of light emitters based on PbS QDs, when observing oxidation enforced shrinking of the active QD volume causing a blue shift of the absorption and PL.

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Abstract 2P (professional, non-award)

QSPRs for melting points of ionic liquids

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Unlike conventional liquids, which consist of neutral molecules, ionic liquids are comprised entirely of ions. Typically, the melting point of ionic liquid falls below ambient temperatures, i.e., it is a liquid at room temperature. Because of their high solubility and extremely low vapor pressure, ionic liquids have found wide application as 'green' alternatives to industrial solvents. Over a trillion different ionic liquids are possible but even basic physical-property data, such as the density and melting point, exist for relatively few. Derivation of melting point QSPRs (Quantitative Structure-Property Relationships) for ionic liquids would therefore greatly aid in molecular design of ionic liquids for specific applications. A series of ten substituted 4-amino-1,2,4-triazolium bromide salts were recently synthesized and their melting points measured. *Ab initio* quantum chemical methods (RHF/6-31G**) were employed to optimize the molecular geometries of the cations of the salts. QSPRs were then derived from quantum chemical, thermodynamic, and electrostatic descriptors. Good correlations with the experimental data were found. Interpretation of the QSPRs in terms of the melting behavior of ionic liquids will be discussed.

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Abstract 3P (professional, non-award)

Measuring Interference-free Coherence Dynamics of Gas-phase Molecules using Spectral Focusing

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Spectral focusing methods with broadband femtosecond pulses have been employed to achieve highly selective measurements in spectroscopy and microscopy. This work will highlight the use of a simplified approach to spectral focusing for selective excitation and detection of gas-phase species. In this approach no adaptive pulse shaping methods are used, instead a simple dispersive element is placed into the beam paths. Additionally, we demonstrate that the use of the spectral focusing method to selectively excite a single species can be coupled with time-resolved measurements, allowing for the observation of interference-free coherence dynamics of the target species despite the presence of additional species. Furthermore, we demonstrate that this method can also be used for gas-phase temperature measurements, making this method ideal for gas-phase measurements of reacting flows and combustion processes.

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Abstract 4P (professional, non-award)

Direct measurements of Raman linewidths of CO₂ S-branch transitions

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We report direct measurements of S-branch Raman-coherence lifetimes of CO₂ resulting from CO₂–CO₂ and CO₂–N₂ collisions by employing time-resolved picosecond coherent anti-Stokes Raman scattering spectroscopy. The S-branch ($\Delta J = +2$) transitions of CO₂ with rotational quantum number $J = 0$ –52 were simultaneously excited using a broadband (~5 nm) laser pulse with a full-width-at-half-maximum duration of ~115 ps. The coherence lifetimes of CO₂ for a pressure range of 0.05–1 atm were measured directly by probing the rotational coherence with a nearly transform-limited, 90-ps-long laser pulse. These directly measured Raman-coherence lifetimes, when converted to collisional linewidth broadening coefficients, differ from the previously reported broadening coefficients extracted from frequency-domain rotational Raman and infrared-absorption spectra and from theoretical calculations by 7–25%.

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Abstract 5P (professional, non-award)

Absorption Spectroscopy Measurements in Harsh Environments using Time-Division-Multiplexed Lasers

Andrew W. Caswell and Sukesh Roy

Spectral Energies, LLC

Scott T. Sanders

University of Wisconsin-Madison

James R. Gord

Air Force Research Laboratory

High-repetition-rate hyperspectral absorption spectroscopy of water vapor has been used to measure gas properties in multiple combustion test articles at the Air Force Research Laboratory. A hyperspectral source is a source that sweeps or cycles through many spectral resolution elements. Although traditional semiconductor sources, most notably vertical-cavity surface-emitting lasers (VCSELs), can be hyperspectral in nature, many new sources have recently been developed, including fiber and free-space designs. Hyperspectral sources can often be easily tailored to operate over a wide range of target wavelengths to achieve a given measurement goal. Of particular interest in combustion diagnostics are techniques that can resolve the temporal profile of the physics of the reacting flow. High-repetition-rate hyperspectral (HRRY) lasers not only include many spectral resolution elements but cycle (in the case of time-division-multiplexed versus frequency-division-multiplexed sources) through them quickly. Typical spectral acquisition rates for such sources are in the range 1–100 spectral resolution elements / μs which permits useful engineering data rates of the flowfield parameters in the 1–100s of

kHz range. For example, cycle resolved gas temperatures and velocities have been inferred in a research-grade pulsed-detonation combustor. The laser source used is termed the TDM 3-FDML because it consists of three time-division-multiplexed (TDM) Fourier-domain modelocked (FDML) lasers. This source monitors sufficient spectral information in the H₂O absorption spectrum near 1350 nm to permit measurements over the wide range of conditions encountered throughout the pulsed-detonation combustor cycle. Absorption-feature Doppler velocimetry was accomplished using a novel counter-propagating beam approach designed to minimize common-mode flow noise.

Received: 2/27/2013

Abstract 1UG (1st undergraduate, award eligible)

**An *Ab Initio* Study of the Products of the SF₂, SFCl and SCl₂
Dimerization Reactions**

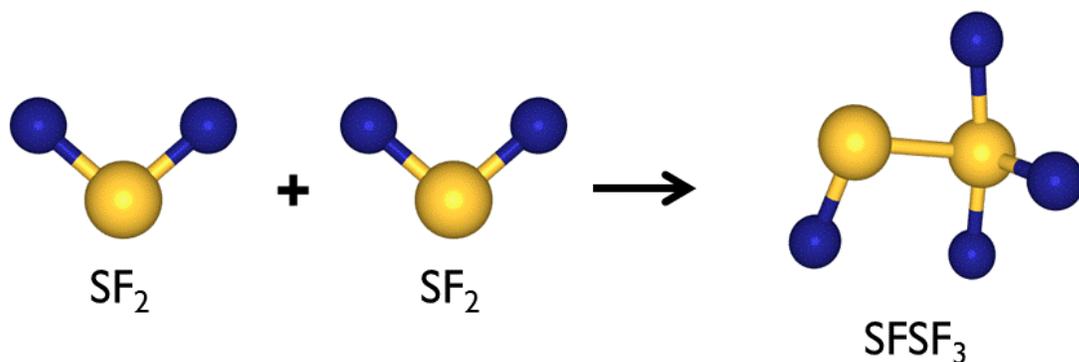
Alaina Engdahl^a, Beth Lindquist^b, Dave Woon^b, and Thom Dunning Jr.^b

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e) Department of Chemistry, University of Illinois, Urbana-Champaign, IL

Recoupled pair bonding theory is a relatively new bonding theory which can be used to describe bonding in hypervalent molecules. The importance of recoupled pair bonds is not just limited to traditionally hypervalent molecules: they are key to the bonding patterns of carbon, boron, silicon, and beryllium.

In this project, single, double and triple Cl substitutions were performed on the SF₂ dimerization reaction, whose product contains recoupled pair bonds (Figure 1). This was done to investigate the cause for the Cl destabilization effect, thereby further developing the recoupled pair bonding theory. The structures for the molecules in this study were optimized using B3LYP/AVTZ and single point energies were calculated using RCCSD(T)-F12/AVTZ. The results suggest that the Cl destabilization effect is not due to steric crowding, but instead is due to the electronegativity difference between Cl and F. The Cl substitutions were found to have a significant impact on the energy and stability of the dimerization product but did not cause any significant differences in the molecular structures.

Figure 1. The SF₂ dimerization reaction



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Abstract 2UG (undergraduate, award eligible)

**Innovative Uses of the Vernier SpectroVis Plus Spectrophotometer
within the General Chemistry Laboratory**

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Using the Vernier SpectroVis Plus Spectrophotometer, three important green chemical concepts were demonstrated: kinetic rate constant, reaction enthalpy, and reaction order determination. To exhibit these subjects, UV reactive threads and beads, color-changing thermal papers, and the Blue Bottle Experiment were observed, respectively. For the threads, beads, and thermal papers, the percent absorbance of white light was utilized, while absorbance decay was observed in the blue bottle system. In regards to the decay constant analysis of the UV reactive threads and beads, each rate constant was calculated by producing first-order kinetics plots of the collected data. Based upon the decay constants, it would seem plausible to assume that there are common dyes/pigments shared between the red and orange threads, the blue and green threads, and none of the beads. Following the completion of the thermal paper experimentation, the enthalpy of reaction for each paper was calculated via Van't Hoff plots collected at six temperatures. Similarly to the UV beads, there did not appear to be any evidence to support shared dyes among the papers. Finally, with respect to the Blue Bottle Experiment, rates of reaction and reagent concentrations were used to determine the experimental reaction orders. It can be noted that using glucose and NaOH concentrations from 0.05 M – 0.20 M, and aqueous methylene blue concentrations from $8.33 \cdot 10^{-6}$ M – $2.50 \cdot 10^{-5}$ M, yielded reaction orders of approximately “one” for the NaOH and methylene blue. However, regardless of the concentrations used, glucose appears to be zero-order with respect to the reaction mechanism.

**Undergraduate Award Applicant

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Abstract 3UG (undergraduate, award eligible)

Comparison of Microcanonical and Canonical Temperatures in Paramagnetic Spin Lattices and Other Two-Level Systems

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Microcanonical temperatures — defined as the “tangential” ($T_{\square} = [\partial U / \partial S_{\square}]_{N,V}$) or “discrete” ($T_{d\square} = [\square U / \square S_{\square}]_{N,V}$) slopes of U vs. S profiles — can be employed in studies of small, isolated and/or non-equilibrium systems. We compare the dependence of T_{\square} and $T_{d\square}$ of paramagnetic spin lattices (PSLs) on magnetic field strength and number of spins N to those of the “tangential” ($T_c = [\partial U / \partial S_c]_{N,V}$) and “discrete” ($T_{dc} = [\square U / \square S_c]_{N,V}$) canonical temperatures. We demonstrate that the sign, magnitude, field- and size-dependence of T_{\square} , $T_{d\square}$, and T_{dc} closely mimic those of T_c , indicating that T_{\square} , $T_{d\square}$ and T_{dc} are legitimate measures of temperature, and that the four temperatures are non-intensive and the microcanonical and canonical entropies S_{\square} and S_c are non-extensive for small ($N \leq 10^{15}$) PSLs. The entropies converge and become extensive in the thermodynamic limit. We detail the origin of the non-extensive entropies, as they indicate that small PSLs violate Boltzmann statistics.

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Abstract 4UG (undergraduate, award eligible)

Electrochemical Detection of Phenol with Metal Oxide Electrodes

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Novel nano materials with biosensing functions possess great potential in the development of a new generation of chemical sensors and actuators in the detection of organic pollutants such as phenol and phenol derivatives. There has been continued interest in the STEM research field to use nanostructured materials such as TiO_2 and ZrO_2 as film forming materials since they have high surface area, optical transparency, chemical inertness, robust mechanical strength, relatively good conductivity, and long term mechanical stability. The goal of this project was to study the novel materials such as TiO_2 , ZrO_2 and mixture ($\text{TiO}_2 + \text{ZrO}_2$) nanoscale modified electrodes to optimize the detection limits of phenol compounds electrochemically utilizing cyclic voltammetry. It will be illustrated that the mixture sol-gel modified electrode gave the best response to phenol. The results of the modified metal oxides/mixture metal oxides will be illustrated by studies such as AFM and SEM as well to explain why the mixture ($\text{TiO}_2 + \text{ZrO}_2$) gave the best results overall due to the morphology.

*Undergraduate student: Miyong Hughes at Wright State University

Received: 3/10/2013

Abstract 5UG (undergraduate, award eligible)

Electrodeposition of Poly-P-Phenylene Conducting Polymer on Different Electrode Materials to Detect 1,2-Dihydroxybenzenes

Miyong Hughes^a, Beth Muir,^b and Suzanne K. Lunsford, Ph.D.^b

Department of Chemistry, Wright State University, Dayton, Ohio 45435, USA

The research interest of the different types of possible electrode materials to undergo Controlled Potential Electrolysis (CPE) with organic conducting polymers such as Poly-P-Phenylene (PPP) were studied on materials of carbon, platinum, and gold electrodes. The PPP were grown electrochemically onto the modified electrode surfaces and utilized to detect 1,2-dihydroxybenzenes such as catechol by cyclic voltammetry (CV). Cyclic Voltammetry (CV) was utilized to determine the stability, longevity, reversibility and diminishing fouling problems typically associated with conductive polymers such as PPP. Fourier Transform Infrared (FTIR) spectroscopy was employed to confirm the modification of the electrode surface (covalent bonding of the polymer) PPP was grown successfully and in the C-H out of the plane para-positioned phenyl groups. The advantages of the PPP-Au electrode to detect 1,2-dihydroxybenzenes will be shown and the stability and longevity will be further discussed as well.

*Undergraduate student: Miyong Hughes at Wright State University

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Abstract 6UG (undergraduate, award eligible)

Evaluation of Chemical Reaction Energies and Barrier Heights

**Darius Lang, Tai-Lyn Wilkerson and Daqing Gao, Central State University,
Wilberforce, Ohio 45384**

Accurate values of chemical reaction energies and barrier heights are essential in understanding thermodynamical properties of chemical processes. Recent study of several approaches for obtaining accurate reactions energies and barrier heights from post Hartree-Fock electronic structure calculations by Truhlar and coworkers suggests that both the gold standard MP2/CBS and CCSD(T)/CBS methods should be used with careful selection of appropriate basis sets. However, it is not feasible to perform CCSD(T) level calculations in many real chemical processes for practical chemists. A new composite protocol, M2.X, which was introduced by Riley and Hobza and coworkers, can produce CCSD(T) level energy differences with dramatic decrease use of computational resources. Here we present our M2.X calculations on the reaction barriers and energies of several organic reactions. The goal of this research work is to assess a number of density function theory models with different moderate basis sets such as 6-311+G(2df,p) in comparison with the accurate wave function based calculations. Some of the DFT methods include B3LYP, M06, M06-L, M06-2X, HTCH, B3P86, B3PW91, B971, wB97X. Useful information will be obtained about the applicability and the development of semiempirical DFT models over the past 15 years.

Acknowledgement:

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Faculty Advisor:

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Abstract 7UG (undergraduate, award eligible)

Thermodynamic Properties of Hydrogen Bonding Complexes

Angel Tartt, David Ross and Daqing Gao, Central State University, Wilberforce, Ohio 45384

Study of hydrogen bonding interactions is important in understanding many fundamental aspects of molecular working mechanisms in biological systems. For example, the genetic information originates from hydrogen bonding interactions in DNA. Molecular level investigation of different hydrogen bonding interaction patterns has been the focus of both experimental and theoretical research. In this presentation, we investigate the interactions of DNA base pair GC and many other dimers of biological interest. We systematically studied the structures of all the compounds involved in this work by a variety of molecular orbital and density functional theory methods, including MP2, MP4 and CCSD(T) calculations with 3-21G, 6-31(G), cc-pVDZ, cc-pVTZ, aug-cc-pVDZ, and aug-cc-pVTZ basis sets. Solvent effects were also investigated. We will present our latest results on accurate evaluations of thermodynamic parameters such as interaction enthalpy and Gibbs free energy which govern the stabilities of real biological and chemical systems at certain temperatures.

Acknowledgement:

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This research is also supported by Ohio Supercomputer Center

Faculty Advisor:

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Abstract 8UG (undergraduate, award eligible)

Presenter: Erin Gallagher
Advisor: Matt Lopper
School: University of Dayton

DNA Replication Restart of *D. radiodurans*

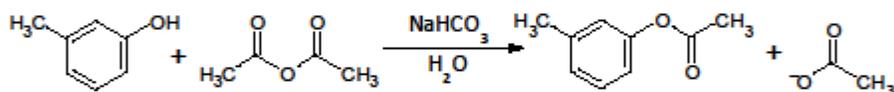
The goal of this research is to study the replication restart pathway of an unusually radiation resistant species of bacteria, *D. radiodurans*. This pathway is used to restart DNA replication after DNA damage has been repaired. Specifically, I investigated the function of an additional 70 amino acid element in the DNA binding domain of *D. radiodurans* PriA. It was hypothesized that there will be a relation between the insert and the radiation resistance seen in *D. radiodurans*. This will be accomplished by cloning the DNA binding domain of *D. radiodurans* priA. The recombinant PriA protein will be analyzed with DNA binding assays. Attempts will also be made to crystallize the DNA binding domain of *D. radiodurans* PriA to obtain a high resolution structural model. It is predicted that the additional sequence in PriA will affect the protein's ability to bind to DNA, and that this difference in binding will partly explain the increased radiation resistance seen in *D. radiodurans*.

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Abstract 9UG (undergraduate, award eligible)

The Computational Determination of Barriers of Decomposition:
Acetylation of *m*-Methylphenol
Kevin Bond, Justin B. Houseknecht*
Wittenberg University

The reaction of acetic anhydride with substituted phenolate ions, nucleophilic acyl substitution, is taught in organic chemistry as a step-wise, addition-elimination process. However, there is evidence that suggests that nucleophilic acyl substitution reactions are not always step-wise, meaning this family of reactions could be concerted, depending on the substituent attached to the phenolate ion. Computational chemistry has been used in order to better determine the energies, geometries, and reaction profile for this process. The reaction of *m*-methylphenolate with acetic anhydride was studied using the 6-31+G** basis set with the MP2, B3LYP, and MPW1K methods. Transition states leading to and away from the two lowest-energy tetrahedral intermediates were found using the QST3 method. All structures were confirmed as minima or maxima using frequency calculations and transition states were additionally confirmed with IRC calculations. Results have shown for the reaction *m*-methylphenol and acetic anhydride the process is a step-wise process. For the B3LYP method, the barriers of decomposition of reactants is 0.7 kJ/mol and products is 5.0 kJ/mol. For MPW1K, the barriers of decomposition are 9.9 kJ/mol and 13.0 kJ/mol, respectively. Other students working on this project using substituents other than methyl have had results consistent with a concerted process.



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Abstract 10UG (undergraduate, award eligible)

Name: Adam Kapuscinski

School: Wittenberg

Abstract

The goal of this research was to quantitatively analyze the level of Raman signal by pyridine on silver colloids due to Surface-Enhanced Raman Spectroscopy. The size of colloids, the concentration of pyridine, the concentration of silver colloids, and the wavelength of the excitation source influenced maximum signal level. The first step in this research was to develop suitable colloids to be used for SERS. Silver nitrate was reduced through the use of different reducing agents[i],[ii],[iii] in order to create different-sized colloids. Colloid size was measured through the use of UV-Vis spectroscopy with absorption wavelengths ranging from 300 nm-800 nm. UV-Vis spectra of each colloid was compared to those from commercially purchased colloids from BBInternational (Table 1). The second step of the research was to prepare the samples for SERS. NaCl (3.2 mM) was added to the colloid solutions prior to SERS in order to effectively adhere pyridine to the colloids. SERS, using a 663 nm wavelength laser, was then ran in two sequences. One, by keeping the colloids at their original concentration while varying the pyridine. A second, by keeping the pyridine constant and varying the colloid concentration. It was found that signal levels increased with increased pyridine concentrations and colloid concentrations, especially sodium borohydride-reduced colloids.

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Abstract 11UG (undergraduate, award eligible)

Conformational Changes for Glucose Binding to the D-galactose/D-glucose-Binding Protein using Molecular Dynamics Simulations

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D-galactose/D-glucose-binding protein (GGBP) works as an intermediate transport protein for glucose and galactose in bacteria, and participates in chemotaxis. As a periplasmic binding protein, it has two conformations: open without ligand and closed with ligand bound. The crystal structures for both the open and closed conformation of GGBP have been solved. Using the center-of-mass pulling algorithm found in the molecular dynamics simulation package GROMACS, the protein is pulled open. The hinge angle and the dihedral twist angle are monitored during the simulations as a way of following the conformational change. We are attempting to separate the sugar-protein interactions from the protein conformational changes to more fully understand the binding process. The free energy difference for the conformational change is determined by using umbrella sampling and the Weighted Histogram Analysis Method (WHAM) in GROMACS.

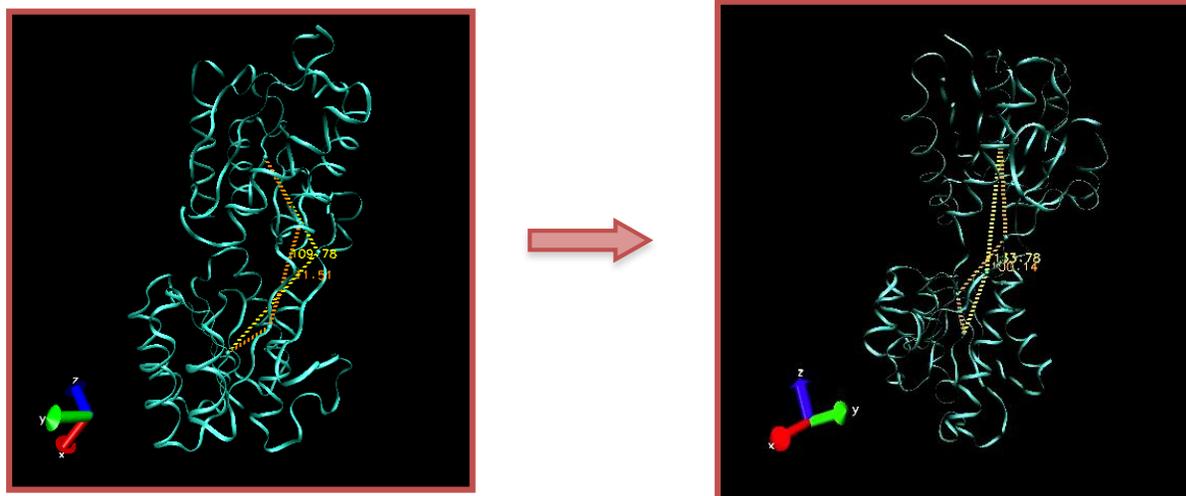


Figure 1. GGBP changes from closed conformation to open conformation (yellow: hinge angle; orange: dihedral twist angle). This figure was made using VMD.

* Undergraduate and competing for awards.

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Abstract 1G (graduate, award eligible)

Monitoring the Health of Glen Helen Nature Preserve:

Fall 2012 Sediment and Water

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Undergraduate students from Wright State University participated in a service learning project to assess water quality at nine sites in the Glen Helen Nature Preserve. The project's water quality assessment goals included analysis of four core areas: on site sampling data (temperature, dissolved oxygen, and pH), microbial data (*E. coli* counts), gas chromatography-mass spectrometry analysis of polar organic contaminants, ion chromatography anion analysis (Cl⁻, NO₂⁻, NO₃⁻, Br⁻, F⁻, SO₄²⁻, and PO₄³⁻), and inductively-coupled plasma chromatography trace metal analysis (Mn, Cd, Fe, Al, Cr, Ni, Cu, Zn, As, and Pb). In addition, sediment samples were collected at three sites for metal analysis as well. *E. coli* and anion levels suggest the Waste Water Treatment Plant is in compliance with its permitted effluent limits for *E. coli* and phosphorus discharge. Nonylphenol-di-ethoxylate and 5 α -androstane are possibly organic contaminants found in the effluent. The Yellow Spring was the only site with metals above the EPA Drinking Limits (As, Fe, and Mn) and the EPA threshold effect concentration limits (As, Cd, Pb). Iron is a naturally occurring metal in the area responsible for the yellow color of the Yellow Spring and like Mn, is considered a secondary contaminant of lesser concern. Low levels of metals may accumulate over time in the Yellow Spring water from natural minerals in the area.

This is possibly the case with As since As was also detected in the Yellow Spring sediment. The presence of Pb probably stems from the lead pipe used in past water system construction work.

** Please consider this abstract for a graduate award at the March 12, 2013 annual poster session.

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Abstract 2G (graduate, award eligible)

**Establishing a global DNA barcode for marine leeches
(*Ozobranchus* spp.) from sea turtles in the Atlantic and Pacific
Oceans**

Triet M. Truong^a, Philip Lavretsky^b, Jeffrey L Peters, PhD^b,
and Audrey E. McGowin, Ph.D.^a

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Marine turtle leeches (*Ozobranchus* spp.) are suspected vector organisms behind fibropapillomatosis (FP), a neoplastic disease plaguing sea turtles. Morphological identification of these leeches can be difficult or impossible due to their small size (ranging from less than 2 mm to 23 mm in length) and various life stages. Character-based DNA barcoding using mitochondrial (mtDNA) cytochrome *c* oxidase I (COI) gene as a molecular marker was employed to identify both species of *O. spp.* (*Ozobranchus branchiatus* and *Ozobranchus margoï*) at all stages of development from turtles in Barbados (five *O. spp.* samples from hawksbill turtles), Florida (43 from green turtles and 13 from loggerheads), Hawaii (34 from green turtles), Hong Kong (two from a green turtle), Brazil (ten from green turtles), and Mexico (two from olive ridley turtles). Molecular analysis of *O.spp.* at other genes (18S rDNA, 28S rDNA, and histone H3) is being used to establish whether Atlantic and Pacific Ocean turtles are infested with cryptic species of *O. branchiatus*. This is the largest molecular data set assembled for *O. spp.* with the most documented number of turtle host species.

** Please consider this abstract for a graduate award at the March 12, 2013 annual poster session.

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Abstract 3G (graduate, award eligible)

Electrochemical Response of Carbon Paste Electrode Modified with Mixture of Titanium Dioxide/Zirconium Dioxide in the Detection of Heavy Metals: Lead and Cadmium

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A novel carbon modified electrode was developed by incorporating titanium dioxide/zirconium dioxide into the graphite carbon paste electrode to detect heavy metals cadmium and lead. In this work, the development of the novel titanium dioxide/zirconium dioxide modified carbon paste electrode was studied to determine the optimum synthesis conditions related to the temperature, heating duration, amount and ratio of titanium dioxide/zirconium dioxide, and amount of surfactant, to create the most reproducible results. Using cyclic voltammetric (CV) analysis, this study has proven that the novel titanium dioxide/zirconium dioxide can be utilized to detect heavy metals, lead and cadmium, at relatively low concentrations (7.6×10^{-6} M and 1.1×10^{-5} M for Pb and Cd, respectively) at optimum pH value (pH=3). From analyzing CV data the optimal electrode's surface area was estimated to be $0.028 (\pm 0.003)$ cm². Also, under the specific experimental conditions, electron transfer coefficients were estimated to be 0.44 and 0.33 along with the heterogeneous electron transfer rate constants of 5.64×10^{-3} and 2.42×10^{-3} (cm/s) for Pb and Cd, respectively.

*Phuong Khanh Quoc Nguyen: Graduate student

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Abstract 4G (graduate, award eligible)

Adsorption Behavior of Polyphenolic Proteins onto High Strength Steel (HY80) and 5083 Aluminum Alloys

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Biopolymers containing chemical groups involved in the formation of adhesive bonds to various substrates (man-made or natural) can be easily found from organisms in nature. The biopolymers utilized by organisms in a process known as quinone tanning contain a unique catecholic amino acid, namely 3,4-dihydroxyphenyl-L-alanine (L-dopa). It has the ability to chelate or couple to the metallic ions or metal oxides that are present at the metal-solution interface. The formation of an insoluble metallo-polymer complex by metal ion bridging at the surface that acts as a stabilizer of the oxide layer can inhibit the process of corrosion. This peculiar capability could be utilized as an environmentally friendly flash rust inhibitor when applied to high strength steels in a humid environment. In the present work, L-dopa containing biopolymers were isolated from the foot of the common blue mussel, *Mytilus edulis* L. There are five L-dopa containing proteins, named *Mytilus edulis* Foot Protein 1 through 5 (MeFP 1 through 5) with a wide range of molecular weights from 6-120kDa. The adsorption characteristics of these proteins onto high strength steel (HY80) and 5083 aluminum alloy were observed. The Bradford protein assay was used to detect the solution concentration of non-adsorbed protein onto either alloy. Langmuir isotherm calculations were made to determine the adsorption behavior based on the differences between the original protein concentration in solution at time zero and the protein concentration in solution at each time point. The optimal solution concentration for maximum substrate coverage onto the metal substrate was then determined. Results and data interpretation for the adsorption studies will be presented and discussed.

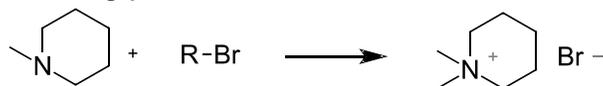
Received: 3/11/2013

Abstract 5G (graduate, award eligible)

Synthesis of N-Methyl-N-Alkylpiperidinium Salts

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Dayton, OH 45435

A series of N-methyl-N-alkylpiperidinium salts has been synthesized by nucleophilic aromatic substitution reaction from N-methylpiperidine and bromopropane, bromobutane, bromopentane, bromohexane and bromoheptane in a Q-Tube setup. The percent yields range from 85 to 92 %. The salts were all ionic solids at room temperature. The N-methyl-N-alkylpiperidinium salts are soluble in dichloromethane. The nucleophilic aromatic substitution products were analyzed by ^1H and ^{13}C NMR, elemental analysis and melting point.



Graduate Student and I would like to be considered for the award.

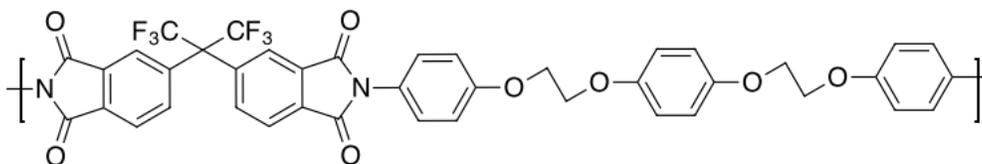
Received: 3/11/2013

Abstract 6G (graduate, award eligible)

Novel Oxyalkylene Polyimides

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Flexible oxyalkylene ether linkages within the polyimide backbone have been shown to decrease T_g but do not have a deleterious effect on thermal stability. We have investigated the incorporation of the 1,4-bis(phenoxyethoxy)phenyl unit into polyimides employing a variety of dianhydrides. The diamine can be synthesized by reaction of p-fluoronitrobenzene with 1,4-bis(hydroxyethoxybenzene) to give the dinitro compound followed by reduction to the diamine by catalytic or chemical hydrogenation. The high melting point of the diamine correlates well with physical properties.



Graduate Student

I would like to be considered for Poster Judging.

Received: 3/11/2013

Abstract 7G (graduate, award eligible)

Nanotechnology and Nanoscience Laboratory Experience at Wright State University

Michelle Edwards,¹ Daniel Foose,¹ Steven Higgins,¹ Jason Deibel,² Hong Huang,³
Sarah Twill,⁴ Ioana Sizemore^{1*}

¹Department of Chemistry, ²Department of Physics, ³Department of Mechanical and Materials Engineering, and ⁴Center for Teaching and Learning, Wright State University, Dayton, OH

Focus: Chemical Education

The National Science Foundation (NSF) has projected that by 2015, the nanotechnology and nanoscience sector will employ ~1 million trained individuals in the United States alone. A team of four faculty from the College of Science and Mathematics and the College of Engineering and Computer Science successfully developed and implemented a novel *Experimental Nanomaterials and Nanoscience* laboratory course (3 credits) that was open to both undergraduate and graduate students. This NSF-funded project aimed to complement currently offered lecture courses, and to train the next generation of nano-scientists and -engineers. The course has raised a lot of interest among students, and the initial class enrollment exceeded the projected expectations. Laboratory modules focusing on the fabrication, characterization and application of nanomaterials were research-inspired and were taught by graduate research students under the direct supervision of faculty. This educational approach improved student's teaching skills and validated understanding of their own research topics. To assess the validity and success of the new course, formative and summative assessments were performed. New evaluation methods and instruments were developed in close collaboration with the Center for Teaching and Learning and the graduate students (e.g., laboratory skill evaluations specific to each experiment module). This new laboratory course was scored highly in the student evaluation forms (e.g., the overall experience in the course was rated 8.75 on a scale from 1 to 10, with 10 being excellent). Entrance and exit surveys indicated that the course held great relevance to students' current field of study and future career paths.

Received: 3/11/2013

Abstract 8G (graduate, award eligible)

Routes to single-molecule SERRS-based detection using concentrated Creighton silver nanoparticles

Kevin M Dorney¹, Joshua D. Baker¹, Austin Williams¹, Adam C. Stahler¹, Seth Brittle¹, Trevor M. Bobka¹, and Ioana E.P. Sizemore¹

¹*Department of Chemistry, Wright State University, Dayton, OH, 45345, United States*

Surface-enhanced Raman spectroscopy (SERS) has been the subject of intense scientific investigation due to its high molecular specificity and extremely low detection limits. SERS-based detection of single-molecules was reported for organic dyes located at the interstitial sites of interacting colloidal silver nanoparticles (AgNPs) under resonant conditions (*i.e.*, surface-enhanced resonance Raman spectroscopy - SERRS). It is well known that the size, shape, and aggregation geometry of AgNPs, along with the excitation wavelength, control the enormous signal enhancements observed in SERS/SERRS. The main goal of this study was to determine the optimum combination of AgNP size and excitation wavelength for single-molecule detection. To achieve this, spherical AgNPs were synthesized via a modified Creighton method, size-selected, and concentrated using a “green” tangential flow filtration approach. Briefly, 4 L of Creighton colloidal AgNPs of 1-100 nm in diameter (14.2 ppm of silver) was filtered down to 10 mL of AgNPs of 6-49 nm in diameter (899.9 ppm) and 50 mL of AgNPs of 50-100 nm in diameter (106.8 ppm). The nanosilver amounts were quantified by inductively coupled plasma optical emission spectroscopy. SERS/SERRS spectra were then collected from the fractionated AgNPs incubated with a Raman reporter, rhodamine 6G, in pre-resonance (632.814 nm) and resonance conditions (532.314 nm), respectively. The largest signal enhancements were obtained using the concentrated AgNPs of 50-100 nm (~64 nm average diameter). The surface enhancement factors (SEFs) were determined to be 2.1×10^6 and 2.64×10^9 in pre-resonance and resonance conditions, respectively, with the latter corresponding to single-molecule detection events.

Received: 3/11/2013

Abstract 9G (graduate, award eligible)

**Tangential Flow Filtration of Colloidal Silver Nanoparticles: A Novel “Green”
Nanotechnology Laboratory Experiment**

Kevin M. Dorney¹, Joshua D. Baker¹, Michelle M. Edwards¹, and Ioana E. P. Sizemore¹

¹*Department of Chemistry, Wright State University, Dayton, OH, 45345, United States*

A novel laboratory experiment was successfully developed for the “green” manipulation of nanomaterials in a cross-curriculum *Experimental Nanomaterials and Nanoscience* laboratory course open to both undergraduate and graduate students. “Bottom-up” nanofabrication methods often utilize chemical modifiers in order to achieve specific control of the spatial dimensions of nanoparticles (NPs), thus generating large amounts of waste and greatly increasing experimental expenditures. Tangential flow filtration (TFF) is an ideal “green” technique for manipulating nanomaterial dimensionality in that, it reduces the amount of auxiliary reagents and allows for real-time analysis of constituent components. Students were introduced to the “green” method of TFF in order to fractionate and to purify Creighton colloidal silver nanoparticles (AgNPs) of moderate size-distribution. Additionally, the setup of two TFF systems (commercial and “home-built”) was an integral part of the experiment that directly involved the problem solving capabilities of the students. Students were able to quantify the size-selection and concentration capabilities of the TFF process by analyzing the ultraviolet-visible (UV-VIS) extinction profile of the localized surface plasmon resonance (LSPR) exhibited by AgNPs. In this laboratory, students became familiar with the fundamental aspects of TFF and its “green” applications for the manipulation of colloidal nanomaterials.

Received: 3/11/2013

Abstract 10G (graduate, award eligible)

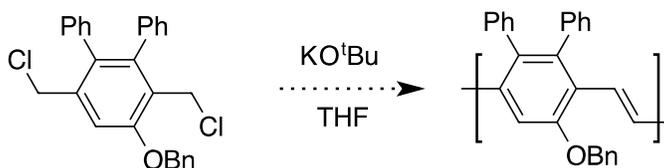
Main Chain Alkoxy/Hydroxy Substituted PPV

Jeremy Lear and William A. Feld

Department of Chemistry

Wright State University

In the interest of the synthesis of polymers that have the potential to possess inherent light emitting properties (LEDs) the synthesis of diethyl 5-benzyloxy-2,3-diphenylbenzenecarboxylate was conducted to produce an intermediate in the synthetic pathway for a novel 1,4-bis(chloromethyl)benzene monomer. The synthesis began with production of diethyl 5-([N-methyliminodiacetato-O,O',N]borane)-2,3-diphenyl-terephthalate, via a Diels-Alder reaction, using 2,5-dicarboethoxy-3,4-diphenylcyclopentadienone and ethynylboronic acid MIDA ester as starting reagents. The diester was oxidized to diethyl 5-hydroxy-2,3-diphenylterephthalate through a reaction with sodium carbonate (Na_2CO_3) and 30% hydrogen peroxide (H_2O_2). Synthesis of diethyl 5-benzyloxy-2,3-diphenylbenzenecarboxylate was achieved through a Williamson ether synthesis involving diethyl 5-hydroxy-2,3-diphenylterephthalate and benzyl chloride. Subsequent reduction of the ester functional groups to alcohols using LiAlH_4 produced 5-benzyloxy-1,4-dihydroxy methyl-2,3-diphenyl benzene. Following the reduction process, the alcohol functionalities were chlorinated with thionyl chloride (SOCl_2) to yield 5-benzyloxy-1,4-dichloromethyl-2,3-diphenyl benzene. The products of each synthetic step were analyzed by ^1H NMR.



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Abstract 11G (graduate, award eligible)

Bis(alkoxyphenyl)cyclopentadienones

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Poly(p-phenylenevinylene) (PPV) has been used in a variety of applications particularly in electronic devices such as LED displays and related semi-conducting systems. Cyclopentadienones have been employed as PPV precursors specifically as carriers of various electron-donating and electron-withdrawing substituents. Alkoxy substituted PPV precursor cyclopentadienones are rare. Dimethoxybenzil or piperil could serve as a basis for synthesizing dialkoxy substituted cyclopentadienones however, its solubility is low in solvents required for cyclopentadiene synthesis. Thus, dimethoxybenzil derivatives were demethylated and alkylated with appropriate solubilizing groups. The reactions and characterization of alkylated benzyl will be presented.

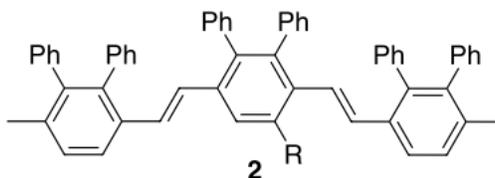
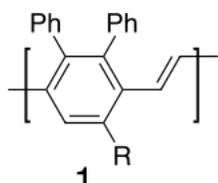
Received: 3/10/2013

Abstract 12G (graduate, award eligible)

Oligomeric Phenylated Poly(phenylene vinylene)s

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Phenylated poly(phenylene vinylene)s (PPV) **1**, have been shown to be efficient LED materials. Among many possible methods, PPV can be synthesized by a phase-transfer catalyzed Wittig reaction involving a phenylated dialdehyde and a phenylated bisphosphonium salt. The polymers produced are fluorescent yellow compounds that glow blue under UV-light. A synthetic approach to well-defined phenylated PPV oligomer **2**, has been defined and carried out.



Please consider the poster for judging.

Received: 3/11/2013

Abstract 13G (graduate, award eligible)

**Quantification of Colloidal Nanosilver by ICP-OES:
A Novel Instrumental Analysis and Nanotechnology Laboratory Experiment**

Jessica L. Fraley, Jessica M. Dagher, Joshua D. Baker, Elizabeth Williams, Steven Higgins, and Ioana Sizemore
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A novel laboratory experiment was developed and successfully implemented for undergraduate and graduate students in *Instrumental Analysis* and *Experimental Nanomaterials and Nanoscience* courses. The main goal of the experiment was to accurately quantify the amount of nanosilver in colloidal suspensions by inductively coupled plasma optical emission spectroscopy (ICP-OES). To accomplish this, students chemically digested Creighton colloids of silver nanoparticles (AgNPs) and quantitatively diluted the samples. Two methods, namely the external calibration method and the standard addition method, were employed for comparative purposes in the quantification of AgNP amounts using a Varian 710 ICP-OES instrument. Students learned that the external calibration method is convenient when matrix effects in the samples are negligible, while the standard additions method compensates for both random and systematic errors. Students constructed then a calibration curve for each method and interpolated the nanosilver amounts. The class average was $15.08 \pm 0.83 \mu\text{g mL}^{-1}$ and $16.28 \pm 3.42 \mu\text{g mL}^{-1}$ for the external calibration method and the standard additions method, respectively. The theoretical yield for the Creighton reaction was $15.42 \mu\text{g mL}^{-1}$. Thus, it was established that matrix interferences in the Creighton colloidal samples are not significant. This laboratory experiment successfully introduced students to the fundamental aspects of ICP-OES and its analytical applications in nanotechnology. Pre- and post-laboratory assignments further improved students' communication and scientific writing skills. Student evaluations revealed a very positive experience with an average overall experiment rating of 9 out of maximum 10.

**I am a graduate student

Received: 3/11/2013

Abstract 14G (graduate, award eligible)

Improving automatic peak parameter determination in crowded NMR spectra by using summit-focused parameter initialization

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- a) Bioinformatics Research Group, Kno.e.sis Center, Wright State University, 377 Joshi Research Center, 3640 Colonel Glenn Highway, Dayton, OH 45435 | (937 - 775 - 5217)

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Nuclear magnetic resonance (NMR) spectroscopists are increasingly being called upon to deal with the spectra of complex chemical mixtures as the utility of NMR in metabolomics is recognized by wider communities. Such spectra often have frequency ranges with very high peak densities, which can approach or exceed the normal resolution of the instrument. These ranges challenge spectroscopic software that estimates the physical parameters of the peaks. We replace the initialization step of an existing peak parameter determination algorithm with one that determines the parameters of one peak at a time focusing only on the part of the spectrum with the most information about that peak – its summit. This yields improvement in the determination of all the fundamental peak parameters: height, location, lorentzianness, and width at half-height on simulated data with a wide variety of peak congestions. The estimate of peak area (crucial to metabolomics) is also improved.

Received: 3/11/2013

Abstract 15G (graduate, award eligible)

NAME: Fadwa G..Constandinidis

ADVISOR: Dr. Eric Fossum

TITLE: Effect of Fluorine Position on the Electrophilic Halogenation of Difluorodiphenyl sulfone Isomers

ABSTRACT: In an ongoing project involving the synthesis of functionalized poly(arylene ether)s that carry pendant phenyl sulfonyl groups, the introduction of an iodo group was desired. The effects of fluorine position on the electrophilic iodination of the 2,4-,2,6-, and 2,5- and 3,5--- isomers of difluorodiphenylsulfone were studied. The relative reactivity, toward EAS, was probed via ¹³C NMR spectroscopy and verified experimentally by iodination with N-iodosuccinimide. The product mixtures and corresponding structures indicated that intermediate stability did not always correlate to reactivity.

Received: 3/11/2013

Abstract 16G (graduate, award eligible)

Presenter: Kyle Knisley – Graduate Student – Wright State University

Kyle Knisley, Daniel M. Ketcha*

Department of Chemistry, Wright State University, 3640 Colonel Glenn Hwy, Dayton,
OH 45435

Abstract

Synthesis of N-substituted-5-fluoro-benzylidene-indoline-2-ones for inhibition of apoptosis

Apoptosis is a highly complex type of cell death in which the cell uses specialized cellular machinery to initiate cell suicide. A family of enzymes is responsible for apoptosis and is known as cystienyl aspartic acid proteases also known as caspases. A new class of small molecule compounds was synthesized to evaluate their ability to inhibit caspases known as N-substituted-5-fluoro-benzylidene-indoline-2-ones. These new compounds have the ability to incorporate three points of variability which increase inhibition of apoptosis. The synthesis of these molecules involved electrophilic substitution of the C-5 position of the isatin nucleus, *N*-alkylation, Wolff-Kishner reduction of the C-3 carbonyl group and Knoevenagel condensation or a new reverse synthesis of electrophilic substitution, Wolff-Kishner reduction of the C-3 carbonyl group, Knoevenagel condensation, and *N*-alkylation. Previous studies with chlorine at the 5-position has shown to inhibit apoptosis in human Jurkat T cells at 10 μ M activity. By using a more electron withdrawing group at the C-5 position (e.g., fluorine) it is believed an increase in inhibition of apoptosis will be observed.

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Abstract 17G (graduate, award eligible)

Quantifying the accumulation of silver nanoparticles in freshwater crayfish tissue by ICP-OES

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¹Department of Chemistry and ²GradPrep Program at Wright State University, Dayton, OH, 45435-0001, U.S.A.

³Department of Environmental Science and Policy, Marist College, Poughkeepsie, NY, 12601, U.S.A.

Silver nanoparticles (AgNPs) are employed in the manufacture of numerous consumer products and research applications due to their unique optical and antimicrobial properties. This extensive use increased the AgNP release into the environment and subsequent exposure of aquatic biota. The main goal of this study was to quantify the Ca content and the amount of Creighton AgNPs accumulated in the exoskeleton tissues of freshwater crayfish by inductively coupled plasma optical emission spectroscopy (ICP-OES). The Creighton reaction is widely-used due to its simplicity, low cost and moderate homogeneity (spherical AgNPs of 1-200 nm). *Procambarus clarkii* was selected as an aquatic model due to its previously demonstrated capability of storing metal ions. Six crayfish per group were habituated in 20 L of river water. Control groups included lab water, Hudson River water, silver nitrate and sodium borohydride reagents. Treatments of 15.3 $\mu\text{g mL}^{-1}$ of AgNPs were administered on the 1st and 7th days of habituation. The crayfish were sacrificed and tissues harvested. Tissues were dehydrated and chemically digested in Optima nitric acid. A set of standards was prepared for Ca and Ag. Ca and Ag concentrations in the exoskeleton tissues were determined through regression analysis using their respective external calibrations. Ag accumulated in the exoskeleton tissue exposed to higher Ag⁺ and AgNP doses. Abnormal mineralization was observed in AgNO₃ and AgNP treatments through histological analysis, in good agreement with the lower Ca contents estimated by ICP-OES. The crayfish readiness for sequestering AgNPs raises major concerns about their implications on human health.

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Abstract 18G (graduate, award eligible)

Microwave-Assisted N-Alkylation of Isatins utilizing DBU

Kyle Knisley, Carly Jordan, Krystyna Wieczerzak and Daniel M. Ketcha*

The N-alkylation of a variety of isatins with alkyl halides can be effected under microwave irradiation in ethanol using DBU as a base. The conditions employed allow for the expedited synthesis of such substrates wherein the products precipitate from the reaction mixture in high yields and high purity after simple filtration. As will be described, microwave irradiation provides a relatively rapid means of effecting N-alkylations of isatin with a variety of benzylic halides, propargyl bromide and ethyl bromoacetate in times ranging from 10-25 min at 140 oC in closed vials. This report involves the first reported use of DBU for this purpose and overall the methods compares favorably with other base-catalyzed alkylations of the isatin nucleus.

Daniel M. Ketcha

Department of Chemistry

Wright State University