FOREWORD
Welcome to the Midwestern Symposium on Undergraduate Research in Chemistry! This symposium is an opportunity for undergraduate scientists, who have been working diligently in their labs, to get together, present their results for the first time, discuss science with other excited researchers, and get a glimpse of the broader scientific community. We have a busy weekend planned, with two poster sessions, a series of talks covering a range of cutting edge research, and tours of various research facilities on the MSU campus. We hope that you will leave this weekend with renewed enthusiasm for your work, fresh ideas, and a new network of friends in science.

ORGANIZING COMMITTEE

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MSU-R:CHEM has been made possible by the generous support of our sponsors:

- Department of Chemistry at MSU
- College of Natural Science at MSU
- Office of the Vice President for Research and Graduate Studies
- Center of Research Excellence in Complex Materials
- MSU Local Section of ACS
### SCHEDULE

#### FRIDAY, OCTOBER 7, 2011

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>3:30 - 4:00 pm</td>
<td>Registration (The registration desk will be open till 7 p.m.)</td>
</tr>
<tr>
<td>4:00 - 4:10 pm</td>
<td>Welcome and Opening Remarks</td>
</tr>
<tr>
<td>4:10 - 4:40 pm</td>
<td><strong>Prof. Greg Baker</strong> (MSU) “Polylactides: from plastics to drug delivery”</td>
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<tr>
<td>4:40 - 5:05 pm</td>
<td><strong>Erica Vogel</strong> (recipient of the 2011 Dye Award in Physical Chemistry) “Expression, purification, and structural studies of viral fusion proteins by solid state NMR”</td>
</tr>
<tr>
<td>5:05 - 7:00 pm</td>
<td>Poster Session I (Undergraduate attendees) / Graduate School Booth</td>
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<tr>
<td>7:00 - 9:00 pm</td>
<td>Dinner</td>
</tr>
</tbody>
</table>

#### SATURDAY, OCTOBER 8, 2011

If you are staying at Gatehouse Suites:
- a complimentary hot breakfast buffet is served beginning at 8:00 a.m. in the gatehouse area off the main lobby
- you need to check out in the morning due to the busy Symposium schedule

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>9:30 - 9:55 am</td>
<td><strong>Steve DiFranco</strong> (recipient of the 2011 Brubaker Award in Inorganic Chemistry) “Single-Site Molybdenum(IV) Mediated Bond Cleavage”</td>
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<tr>
<td>9:55 - 10:20 am</td>
<td><strong>Hong Ren</strong> (recipient of the Harold Hart Award in Organic Chemistry 2011) “Direct Catalytic Asymmetric Aminoallylation of Aldehyde – Synergism of Chiral- and Non-Chiral Brønsted Acids”</td>
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<tr>
<td>10:20 - 10:30 am</td>
<td>Group photo</td>
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<tr>
<td>10:30 - 12:30 pm</td>
<td>Poster Session II (presented by grad students)/Tour of instruments</td>
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<tr>
<td>11:30 am - 12:30 pm</td>
<td><strong>Faculty gathering (room 481)</strong></td>
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<tr>
<td>12:30 - 2:30 pm</td>
<td>Lunch/Tour of campus</td>
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<tr>
<td>2:30 - 2:55 pm</td>
<td><strong>Li Cui</strong> (recipient of the Babcock Award in Analytical Chemistry 2011) “Evaluation of factors affecting phosphate group scrambling during CID-MS/MS”</td>
</tr>
<tr>
<td>2:55 - 3:25 pm</td>
<td><strong>Prof. Elke Schoffers</strong> (Western Michigan University) “Enzymes for the preparation of B-ring functionalized 1,10-phenanthroline derivatives”</td>
</tr>
<tr>
<td>3:25 pm</td>
<td>Presentation of Awards and Closing Words</td>
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### REGISTRATION AND PARKING

The Registration Desk will be located in the lobby of the Chemistry Building.
Free parking permits will be provided at the Registration Desk. Parking is available in Lot 41 and the Shaw Lane Parking Ramp, right across S. Shaw Lane from the Chemistry Building. Parking permits are not needed after 6 pm, nor on weekends.

### EVENT LOCATIONS

**Presentations:** Room 136 Chemistry Building
**Poster sessions:** Chemistry Building 1st Floor Hallway
**Dinner on Friday:** Room 481 Chemistry Building
**Lunch on Friday:** The Gallery at Snyder/Phillips (-0.5 mi) or Brody Square (-1.3 mi)
## LIST OF PARTICIPANTS

### Undergraduate Attendees

<table>
<thead>
<tr>
<th>Name</th>
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## Faculty Attendees

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<td>Baldwin, Bruce</td>
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Abstracts

1A

Computational Investigation of a Proposed DNA Checking Site in Klentaq DNA Polymerase I

Sarah Graham, Andrés Cisneros
Chemistry Department, Wayne State University

High fidelity DNA replication is necessary to preserve the integrity of an organism. Incorrect replication may lead to diseases; therefore discovering the ways in which organisms achieve such high fidelity replication is of interest. Recently, a novel post-insertion checking mechanism has been proposed where the newly inserted nucleotide is translocated to a putative checking site (1). This checking site is located one base down from the DNA insertion site and is responsible for checking that the correct DNA base has been inserted opposite the template strand. In order to investigate this proposed checking site, we performed computational simulations of correctly and incorrectly paired DNA sequences in both the pre-insertion and checking site positions. Energy decomposition analysis was performed on the resulting trajectory, revealing residues that may be involved in the checking site. To further study these residues, non-covalent interaction analysis was also performed. We will discuss several residues resulting from these analyses that may be involved in the proposed checking site mechanism.


1B

On the Reaction Mechanism of Na, Mg and Al with Water

Nicholas A Fisher and Daniel B. Lawson
University of Michigan-Dearborn

A theoretical study of the reaction of sodium, magnesium and aluminium with gas phase water was performed with Density Functional Theory of the B3LYP and M06 types with 3-21g, 6-31g* and 6-311++g** basis sets. Our results indicate 3 possible reaction pathways that involve several isomers. The enthalpy of formation for the reaction between the metals and water at 298 K are calculated. Some results are in good agreement with experiment and with previous studies.
2A

**Single Shot Pulse Measurement**

**Nathan Butcher, Shreya Nad, Vadim V. Lozovoy, Marcos Dantus**  
**Michigan State University**

As laser systems capable of producing ultrashort pulses become available, the need to measure these kinds of pulses increases. Among the best pulse characterization methods available today is Multiphoton Intrapulse Interference Phase Scan, or MIIPS. It works by using a known reference phase to directly measure the second derivative of the phase, which is what is responsible for any temporal distortions in the pulse.\(^1\) MIIPS has been shown to be extremely accurate for measuring the dispersion of optical materials such as glass and quartz as well as gases and liquids. The next frontier would be to measure how the optical properties of such materials are modified when an intense pulse transmits through them. Unfortunately, MIIPS cannot measure transient changes. Typically it takes several seconds to complete the measurement, making the method impractical for probing transient dispersion.

The project that I am working on is to obtain a single shot measurement of the pulse by recording the second harmonic spectrum of a laser. A sinusoidal phase is applied to the pulse, causing the second harmonic spectrum to split into two peaks. For every single laser shot, movement of these peaks can be used to determine deviations in the dispersion experienced by the probe laser pulse as a function of time delay from the intense pump pulse that preceded it. Analysis of the spectra collected as a function of time will yield will yield the transient changes in dispersion induced by the pump pulse.


2B

**Revealing Molecular Dynamics Through DC Slice Ion Imaging**

**Niclas A. West, Michelle L. Warter, Michael P. Grubb, Simon W. North, and Jeffrey A. Bartz**  
**Department of Chemistry, Texas A&M University, College Station, Texas 77842, United States**  
**Department of Chemistry, Kalamazoo College, Kalamazoo, Michigan 49006, United States**

Velocity mapped ion imaging is a well-established technique for studying photolysis dynamics on the molecular level. Mapping the velocity of a spherical cloud ensemble of photofragments provides enough information to characterize how the fragment velocities, angular momenta, and transition dipole moments are correlated during dissociation. Here we dissociate methyl nitrite with 355 nm linear polarized light, probe the NO fragments with a \(1+1\)’ REMPI scheme, and velocity map the NO\(^+\) fragments to learn where photodissociation reaction energy is partitioned. Conventional ion imaging maps the NO\(^+\) ions by sending the 3D Newton ion sphere via \(>2\) electrodes toward a 2D microchannel plate (MCP)/phosphor detector to be crushed into a 2D image. The newer DC slicing technique uses \(>3\) electrodes of a special ratio 1:0.93:0.81:0.75 of voltages to elongate the Newton sphere several hundred ns along the time of flight axis. The MCP is then gated by application of a voltage pulse to accept only \(-40\) ns of the center of the elongated Newton sphere. This collects only the central slice of the Newton sphere. A sliced ion image has the advantages that the bipolar moments can be determined without the need for mathematical deconvolution and that fitting a 2D distribution is much simpler. Disadvantages of DC sliced images is that much of the Newton ion sphere (signal) is thrown away and that the lower electrode voltages used make the ions more susceptible to stray fields.
The Interaction of Graphene Oxide with H₂

Marjorie M. Bridgewater and Daniel B. Lawson
University of Michigan-Deaborn

Graphite, the stuff inside pencils and dry lubricants, consists of a series of layers of carbon atoms bonded together in 2 dimensional lattices. Graphene is a single layer or monolayer of graphite. Graphene oxide (GO) is the oxidized form of graphene and has recently indicated value in catalytic processes such as the oxidation of alcohols and alkenes as well as alkyne hydrations. Unlike the more commonly used metal materials, the carbonaceous nature of the graphitic material make GO much more environmentally friendly. This work uses Density Functional Theory to study how GO interacts with H₂ and the OH groups of alcohols.

Benzene Chromium Tricarbonyl: Ultrafast Dynamics of a Molecular Rotor

Ian Nilsen, Kevin Kubarych
University of Michigan

The spectral location of metal carbonyl stretches in the infrared near 2000 cm⁻¹ make promising vibrational labels to probe the dynamics of proteins and other complex biological systems. One such metal carbonyl compound, benzene chromium tricarbonyl (BCT), was complexed with β-cyclodextrin as a model for molecular recognition and nanoconfinement. Using photodissociation and FTIR spectroscopy, we identified two distinct conformations of the inclusion complex, with the carbonyl ligands alternatively solvent exposed or embedded within the β-cyclodextrin cavity. To access equilibrium solvation dynamics and assess its suitability as a dynamical probe, benzene chromium tricarbonyl was studied using 2DIR spectroscopy. 2DIR spectroscopy is an ultrafast technique that provides direct frequency dynamics information that is generally hidden in one-dimensional spectra. The 2DIR data showed signatures of the ultrafast torsional rotation of the piano-stool BCT complex in non-polar long-chain alkanes. The relative simplicity of the BCT system makes it amenable to treatment with a simple one-dimensional model. A periodic potential function corresponding to the torsional potential energy surface was calculated using quantum chemistry. Consistent with previous work, we identified two stable isomers: an eclipsed structure, where the carbonyls lie directly under the hydrogens of the benzene ring and a more stable staggered structure, where the carbonyls are rotated 30° from the eclipsed structure. The barrier to rotation from the eclipsed to staggered structure was estimated at 0.3 kcal/mol. We used this potential function to parameterize a one-dimensional Langevin dynamics simulation of the torsional motion, with solvent viscosity as the sole input. Gaussian white-noise and Gaussian-Markov approaches were compared to see what effect correlating the random fluctuating torque would have on the simulation. The trajectory output was then mapped to frequencies, based on further quantum chemistry simulations which showed that the vibrational frequency of the carbonyl stretches varied by 10 cm⁻¹ between the two isomers. The frequency-frequency correlation function was then computed and fit using a biexponential decay to compare with 2DIR measurements. To directly compare the results of our simulations to experiments, a series of 2DIR spectra of BCT were recorded in various viscosity solvents prepared using hexane-squalane mixtures. In general we found that the 1D model with essentially no adjustable parameters could predict the reaction-associated spectral diffusion timescales very well. This work represents the first observation with 2DIR spectroscopy of internal reaction dynamics approaching the “fast-exchange” limit.
4A

Laser Optimization for Biomedical Imaging of Full-body Organisms

Kristen Zuraski, Ilyas A. Saytashev, Sergey N. Arkhipov, Nelson S. Winkler, Vadim Lozovoy, Marcos Dantus
Department of Chemistry, Michigan State University

Providing real-time biopsy information without cutting tissue will one day become a common procedure within the medical field that will eliminate the need for more traditional invasive procedures. This work is relevant to nonlinear optical microscopy, a modality that has become quite popular. Typical of any practice that is expected for widespread use, however, there is a need to perfect this method in regards to minimizing the harm to the sample while still being able to obtain quality images. In some cases, the laser can result in subsequent cell death. Therefore, it is necessary to determine safety parameters that will insure cell integrity. In order to achieve this, experiments with varying time durations were performed on *Drosophila melanogaster*, which are a convenient model for our experiments due to its easy cultivation, size, and relatively short lifespan. Its complete transformation between developmental stages also allows us to separate the immediate damage that occurs to the larvae during irradiation from the DNA damage that can be observed after the larva transforms into the pupae and later the fly form. My current experiments involve irradiating larva and then immediately photographing them to observe the differences in the initial damage as a function of the pulse duration. Specifically, we investigate the effects of lasers with different pulse durations of 37 and 100 femtoseconds, on whole-body, living organisms. This data will later be added to what we observe in terms of DNA damage, which will also be compared to our previous data on the lethality rates of the organisms. The totality of these experiments will then allow us to draw a conclusion as to the optimal laser parameters for imaging in terms of the safety of the organism.

4B

Modeling the Interface between Islet Amyloid Polypeptide and Inhibitors of its Aggregation

Hector Figueroa, Dr. Maria Milletti
Eastern Michigan University

Human islet amyloid polypeptide (hIAPP) forms cytotoxic plaques in the pancreases of Type II Diabetes patients. Preventing formation of these aggregates is a potential treatment for this disease. Since insulin itself inhibits these plaques from forming, a series of insulin-based inhibitors have been synthesized and assessed for their ability to inhibit fibrillogenesis. In this study, we examine the interface between each inhibitor and hIAPP using Density Functional Theory in an attempt to understand the underlying mechanism of interaction between the molecules and assist in designing more potent inhibitors. Overall, each inhibitor displayed a variety of unique non-specific, hydrogen-bonding-like interactions. Additionally, those inhibitors possessing a Glutamate residue were able to form a strong association with the Arginine-11 side chain of hIAPP. Comparison with experimental data suggests inhibitory capability depends on the strength of the salt bridge and the ability of the compound to bind along the 11-16 region of hIAPP.
The Effects of Delignification by Catalytic Oxidation in Iron(III)-Tetraphenylporphyrin and Iron(III)-Phthalocyanine

Charles Chen1,2, Zhenglun Li1, Dr. Chi-Kwong Chang2, and Dr. David Hodge1
1Department of Chemical Engineering and Material Science, Michigan State University
2Department of Chemistry, Michigan State University

Lignin is a complex compound in the secondary cell walls of plants, and it has negative effects to biofuel productions made from lignocellulosic biomass. Catalytic oxidation is a method of using transition metal-catalyst and hydrogen peroxide that can be applied to paper bleaching. Many studies have mentioned that this solution could be used to oxidize the lignin polymers and modify the structure of biomass producing biomaterials from starch, cellulose and lignin. Iron(III)-tetraphenylporphyrin [Fe(III)TPP] and iron(III)-tetrakis(pentafluoro-phenyl)porphyrin [Fe(III)TFPP] are effective metal-catalysts in catalytic oxidation. In Fe(III)TFPP, the electrons withdrawn by fluorides on phenyl rings would reduce the electron density in active center and increase the interaction of iron(III) with hydrogen peroxide. The cost of metalloporphyrin is an important issue, so Iron(III)-Phthalocyanine [Fe(III)Pc] is an ideal porphyrin-like catalyst that has cheap and easy preparation hence reduces the cost in the biofuel production. The benefits of this method are using less energy and chemicals to achieve high efficient in delignification. The catalysts and catalytic oxidations would be studied with lignin models and biomass by UV-spectrometry, size-exclusion chromatography, lignocellulosic biomass composition analysis, and enzymatic digestibility. Therefore, molecular modifications of the compounds help us to design better transition metal catalysts in delignification, and broaden the application of catalytic oxidation in biorefinery.

Comparing the Sorption Behavior of Veterinary Antibiotics onto Various Environmentally Relevant Surfaces using Surface-Enhanced Raman Spectroscopy (SERS)

Mallory J. Schweitzer and Matthew A. Young
Hillsdale College

The focus of this project was the adsorption of the veterinary antibiotic cephapirin onto environmentally relevant surfaces, studied using surface-enhanced Raman spectroscopy (SERS). To mimic an environmental surface, we deposited alumina on silver film-over-nanosphere substrates (AgFON) using atomic layer deposition (ALD). Studies were also performed on uncoated nanostructured AgFON surfaces to serve as a control. This was to verify that the spectra obtained from various compounds on the ALD alumina coated AgFON substrates were not from the compound getting through deformations in the substrate to the silver. We also coated the substrates in various organic monolayers using thiol chemistry to mimic humic substances found in soil. The sorption behavior of cephapirin, 7-acetocephalosporonic acid, benzenethiol, sulfamethazine, and benzoic acid were characterized in contact with alumina, silver, and several organic moieties. Cephapirin was found to bind irreversibly to every organic monolayer, as the peaks of the spectra did not significantly decrease after multiple washings of the substrate, or after letting the substrate dry completely and re-submerging in water. To better determine the binding mechanism of cephapirin, we studied pyridine because it is currently thought that cephapirin binds through the pyridine ring. This yielded results that show that cephapirin must bind to a surface through more than just the pyridine ring. Sulfamethazine was used as a comparison drug, and reversible binding was seen on every substrate and monolayer.
6A

Determining the Pressure inside an Intact Carbonated Beverage Can & Possible Clathrate Formation

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This experiment combines Henry’s law and freezing point depression measurements in order to calculate the \( P_{\text{CO}_2} \) inside unopened carbonated cans/bottles. The combined equation:

\[
P_{\text{CO}_2} = \frac{\Delta T_{fp}}{k'_n k'_p}
\]

allows for the estimation of \( P_{\text{CO}_2} \) of carbonated water, by simply measuring \( \Delta T_{fp} \). The experiment is performed by using black electric tape to attach Microlab thermistor sensors to the outside of unopened cans of sparkling water and to opened rinsed cans that are filled with deionized water. The cans are then placed in a freezer at \(-15^\circ C\). The temperature of each fluid is measured over time. Upon freezing, the supercooled liquids warmed and levelled off at their freezing temperatures; allowing the calculation of \( \Delta T_{fp} \) to be made.

While performing this experiment, it was observed that the unopened carbonated beverage containers sometimes exploded when they were frozen below a certain temperature, but the non-pressurized counterparts did not exhibit the same phenomena (no explosion and less physical space seemed to be taken up by the resultant ice formation). And so, \( \text{CO}_2 \) clathrate formation may be occurring at these lowered temperatures. FTIR data as well as temperature versus time data are provided as possible evidence in support of \( \text{CO}_2 \) clathrate formation.

6B

Exploring the Orientation of Photoproducts Using Circularly Polarized Light

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Methyl nitrite is a highly studied molecule for investigation of the photodissociation dynamics of a bent system. While our lab has previously studied the vector correlations in 225 nm photodissociation of \( \text{CH}_3\text{ONO} \), revealing the alignment of the \( J, v, \) and \( \mu \) vectors, the orientation of these vectors has not yet been measured. The goal of this investigation was to discover the orientation of the \( J \) vector in nascent NO to determine whether the O–NO bond angle increased or decreased during the dissociation event by measuring the value of the \( \beta_0^2 \) odd bipolar moment. A three color photodissociation and ionization; 280 nm linearly polarized light for dissociation of \( \text{CH}_3\text{ONO} \), a tunable 223 – 226 nm circularly polarized beam to probe the NO, and a linearly polarized beam for ionizing the excited NO. The \( \text{NO}^+ \) product ions were detected by photofragment ion imaging. The ion images were analyzed in order to determine the value of the \( \beta_0^2 \) odd bipolar moment. For \( P \) and \( R \) branch transitions, the ion images showed a qualitative dependence on the helicity of the circularly polarized probe beam and produced average values of \( \beta_0^2 \) of -0.40 and -0.23 for \( P \) and \( R \) (\( P_{11} \) and \( Q_{21} + R_{11} \)) branches respectively. As expected, the \( Q \) branches showed no significant dependence on the helicity of the probe light. These values indicated that the O–NO bond angle increases on the excited surface. This result is in contrast to \( \text{NO}_2 \), which has been shown to have the O-NO bond angle decrease as the dissociation event unfolds.
7A

Photovoltaic Devices Based on Porphyrin Polymeric Donor Materials: A Computational Study of Linker Effects

Zachary L. Dunn*, Morgan A. Hammer, Trilisa M. Perrine
Ohio Northern University

The electronic properties of porphyrin based polymeric systems for use in organic photovoltaic (OPV) devices were studied using DFT with the B3LYP functional and the LANL2DZ basis set. The focus was upon the exploration of using polymers based on porphyrin as donor molecules in the OPV donor-acceptor regime. The goal was to minimize the gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) in order to optimize the wavelengths and amount of incident light the OPV devices absorb. A variety of possible linker moieties between the porphyrin molecules were explored, including ones based on thiophene and furan heterocycles, phenyl rings, and butadiyne functional groups and which included single, double, or triple bonds between the porphyrin ring and the linker core. The most promising of these included two thiophene heterocycles and two triple bonds.

7B

Effects of the Molecular Conformational Changes of N,N-dimethyl nitrosamine \((\text{CH}_3)_2\text{NNO}\) on Vector Correlations

Masroor Hossain, Aidan Klobuchar, Jeffrey Bartz

Department of Chemistry, Kalamazoo College

Photodissociation dynamics investigate the microscopic details of chemical reactions. We carried out an investigation to determine whether a predicted conformational change in the excited state of N,N-dimethyl nitrosamine (DMN) will result in a propeller-like trajectory of the ejected NO product. DMN was photodissociated at 355 nm in a velocity-mapped ion imaging apparatus. Vector correlations between and among the transition dipole, angular momentum, and velocity were measured. The correlation between the velocity \(\mathbf{v}\) and angular momentum \(\mathbf{J}\) in DMN was almost zero. This could be explained because the N-N bond stretched and a conformation change occurred where NO puckered toward the methyl groups upon excitation. We speculated that NO rotated out of the plane of the molecule having both propeller- and Frisbee-like motions.
8A

Validation of Multi-State Lambda Dynamics Free Energy Method for a Series of Inhibitors of Dihydrofolate Reductase

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Traditional free energy calculations require time-intensive simulations and are usually evaluated for pairs of compounds. Multi-Site \( \lambda \) Dynamics (MS\( \lambda \)D) is a computationally-efficient strategy for obtaining accurate free energy estimates for series of congeneric compounds in a single simulation. In this study, hydration free energy and binding affinity estimates are computed using MS\( \lambda \)D in the CHARMM macromolecular simulation program for a series of 24 trimethoprim-like inhibitors (TMP) of dihydrofolate reductase (DHFR). These calculations rely on automated parameter assignments obtained from MATCH and optimized biasing potentials. The resulting relative free energy estimates correlate well with experimentally obtained values and with estimates obtained from traditional free energy perturbation calculations. The study of this DHFR-TMP system highlights the efficiency of MS\( \lambda \)D simulations and demonstrates the usefulness of MS\( \lambda \)D as a beneficial tool for modelling drug-protein interactions and accelerating drug discovery processes.

8B

Investigating the Sorption of the Veterinary Antibiotic Cephapirin on a Model Soil Surface using Surface-Enhanced Raman Spectroscopy (SERS)

Paul D. Schmitt and Matthew A. Young
Hillsdale College

Surface-enhanced Raman spectroscopy (SERS) has been used to investigate the molecular details of the sorption behavior of the veterinary antibiotic molecule cephapirin on model soil surfaces. SERS measurements on environmentally relevant mineral oxides are made possible by coating nanostructured Ag SERS-active substrates with sub-nanometer thin films of alumina using atomic layer deposition (ALD). The surface binding mechanism of cephapirin has been investigated by comparing the sorption behavior on both ALD alumina coated substrates and bare Ag substrates. The sorption behavior of pyridine has also been characterized in order to serve as a comparison. While it is notoriously difficult to achieve quantitative results using SERS, a robust protocol has been developed to acquire adsorption isotherms from SERS measurements in aqueous solutions on our ALD alumina coated Ag substrates. Adsorption isotherms, and corresponding binding constants calculated from a Langmuir adsorption model, are reported for cephapirin on both alumina and Ag and pyridine on alumina. It was found that cephapirin binds strongly to both alumina and Ag surfaces, with the binding to Ag being stronger. The interaction of the cephapirin molecule with alumina is found to be mostly through the pyridine ring on the molecule. The implications of the data for the transport and bioavailability of cephapirin in the environment are discussed.
The Application of Molecular Dynamics Simulations to Study the Monomeric and Dimeric Forms of Islet Amyloid Polypeptide

Michael J. Robertson, Dr. Charles L. Brooks III
University of Michigan, Department of Chemistry and Biophysics Program

The formation of deposits of aggregated insoluble Amyloid peptide fibrils is a common hallmark of many diseases, with at least 27 distinct fibril peptides discovered and at least 19 associated diseases. As aggregation is primarily a biophysical phenomenon, driven by intermolecular forces and/or entropic effects, we have explored the use of Molecular Dynamics techniques to study various aspects of the structure and dynamics of monomers and dimers of IAPP; the amyloid peptide that forms the fibrils associated with Type-2 Diabetes. Particularly important to our approach was the implementation of a Gouy-Chapman double layer electric potential to accompany the GBSW implicit membrane model in the CHARMM force field package to allow for simulations of peptides in an anionic lipid environment; which is thought to be crucial for the folding and oligimerization of many amyloid peptides.

By combining this anionic membrane model with All-Atom Replica Exchange Molecular Dynamics, we produced results which suggested that the anionic character of membranes increases the binding strength of the peptide to the membrane, as predicted by experiment, as well as influencing the structure of the N-terminal helix associated with the membrane disruptive properties of IAPP. Additionally, our results were able to provide insight into how factors such as pH and amidation of the C-terminus, which are known to affect peptide function and fibrilization affect the structure of the membrane bound state. Finally, we were able to produce several possible dimer structures, which suggested two different types of dimer association.

Conductimetric Titration of Alginate Gels

Christopher Thiebaut
Spring Arbor University

Alginate gels have, in addition to their food uses, potentially significant application for long-term treatment of diabetes by protecting injected insulin-producing cells from the host’s immune system without the need for immunosuppression. This work quantitatively explores the gram-to-mole ratios with which Sodium Alginate will react to form gels when dropped into a solution containing known quantities of specific metal cations. Results indicate that the gram-to-mole ratios are broadly consistent with the difference in charge between different metal cations. In addition to the charge of the cation itself, other factors which may impact the apparent ratio of alginate to cation are the presence of different anions in solution and the physical stir rate of used during the reaction, which may impact the amount of unreacted alginate that is trapped inside a mass of alginate and prevented from reacting with the cations in solution.
Molecular Dynamics Simulation of the Condensation Coefficient of Water

Patrick Louden, Ryan Shoenborn, Christopher Lawrence Ph.D.
Grand Valley State University

Experiments have found the condensation coefficient for water condensing onto pure water to be between 0.1 and 1 with more recent experiments having found a value of 0.2 ± 0.1. However, molecular dynamics simulations of water result in a condensation coefficient of 1. These deviations could result from assigning condensed phase parameters to the bulk, surface, and gas phase water molecules in the simulations. We varied the charges and the Lennard-Jones parameters for a gas phase water molecule in a condensation simulation using the SPC/E model. We have concluded that to obtain a simulation condensation coefficient of 0.2, unrealistic parameters must be assigned to the water molecules.

Linking Disease Phenotypes to their Structural Consequences in any Given Protein: A Novel Bioinformatics Method for Analyzing Cohort Genotyping Data

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Bioinformatics has bestowed an abundant amount of information regarding complete-genome genotyping across phenotype cohorts. The resulting data, however, is disorderly and difficult to interpret. The method of depositing single nucleotide polymorphisms (SNP’s) generally results in files that are too large and in many cases unmanageable. We have created an algorithm that incorporates sorting very large SNP lists, and traces them back to their ultimate position in the protein sequence. This allows us to search across phenotype cohorts for mutations that cause a change in protein sequence. Using this method, we correlated eight phenotype cohorts to DNA polymerase mutations. Our algorithm found 67 SNP’s within the DNA polymerase genes. Mutations in the polymerase protein product were found in 39 out of the 67 SNP’s. Not only has this process productively correlated cancer phenotypes to mutations in human DNA polymerases, it is adaptable to basically any system.
11A

Graphene Oxide: A Computational Study of Structure and Related Properties

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Recent literature indicates Graphene Oxide (GO) to behave favorably in certain catalytic processes and have applications as sensitive chemical detectors. Unlike more commonly used metals in catalysis, the carbonaceous nature of the graphitic material make GO more environmentally friendly. While of a central theme in many studies, not much is understood about the structure of GO. Graphene oxide is known to consist of various carboxylic and epoxide functional groups attached to the surface of graphene with various orientations. This work uses *ab initio* modeling to study the various aspects of proposed structures of GO to investigate the nature of the electronic structure and relative stability of various isomers. We compare available experimental data from the literature with our computationally generated results to better assess the topography of GO.

11B

Computational Study of Substituent Effects on the Band Gap of Porphyrin Based Polymeric Systems

Morgan A. Hammer*, Zachary L. Dunn, Trilisa M. Perrine
Ohio Northern University

Porphyrins have electrical properties that may be utilized as donating materials in photovoltaics. A computational study (DFT with B3LYP and the LANL2DZ basis set) was performed on functionalized zinc-centered porphyrin monomers with the goal of lowering the HOMO/LUMO gap. By narrowing the band gap, a greater portion of the solar spectrum can be absorbed. Two different substituents that are known to improve porphyrin solubility were tested for their contribution to the band gap. It was determined that their contribution is small, and that these substituents may be truncated as an adequate approximation for more extensive oligomer calculations. The electron donating and electron withdrawing groups, -NH₂ and -NO₂ respectively, were tested in various combinations at the beta and meso positions. Both substituents proved to lower the band gap, with the amino groups proving most effective at the meso positions and the nitro groups proving most effective at the beta positions.
Reduction of Acetophenones using NiAl Metal Clusters

Taavi Vint and Daniel B. Lawson
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Many synthesis reactions in organic chemistry are catalyzed by heavy metals such as Pd or Rh or by some complex ligated heavy metal. Due to the cost and short lifetime of the catalyst, these processes are not conducive to industrial scale-up. Lighter, more environmentally friendly metals can also catalyze reactions so long as an additional energy source is provided. Several recent studies report that microwave radiation can accelerate such relevant organic reactions, thus lowering cost and leading to more environmentally friendly pathways. This work models the reduction of acetophenones using Ni-Al alloy catalyst to give the corresponding alkylbenzenes. The Ni-Al metals are modelled as small clusters and the reactions are in the gas phase, but the potential energy landscape suggests that minimal energy would be required to produce favorable results.

Modification to the Temple Bound Method

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Department of Mathematical Sciences, Indiana University South Bend

In 1935, George Temple derived a formula for calculating lower bounds to compliment variational upper bounds to the ground state energy of a quantum system. In this project we studied both the Hydrogen Atom and the Quantum Harmonic Oscillator and introduced a slight modification to their Hamiltonian Operators. Although seemingly simple at first glance, the modification proved to work best for trial functions that poorly approximate the true ground-state wave function.
13A

Computational Design of Phosphafluorenes in Optoelectronic Applications through Chemical Substitution

Jacob Smith, Heidi Phillips, Pavel Anzebacher, Barry Dunietz
University of Michigan

Phosphafluorenes exhibit unique optoelectronic properties that can be used to advance related applications. The Phosphafluorenes can be tuned by chemical substitutions to serve as hole or electron transporting materials. We use quantum chemical modeling calculations to gain further insight on their properties and to guide their design. We analyze the effect of bromination on the mobility of substituted phosphafluorenes. We employ recently developed range separated hybrid (RSH) functionals in density functional theory (DFT) and time-dependent (TD)-DFT based modeling of the ground and excited electronic states. The success of the RSH functional to reliably describe the mobility properties is demonstrated by benchmarking against available experimental data. Predictions of new designed molecules are then provided to direct the synthesis and device fabrication efforts.

13B

Investigations into the Reactivity of Biomimetic Nonheme Oxoiron(IV) Intermediates with Hydrogen Peroxide

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High-valent oxoiron(IV) intermediates found in the active sites of nonheme metalloenzymes have been extensively studied recently due to their significance in organic oxidation reactions in nature. To gain a greater understanding into the mechanistic pathways of these oxidation reactions, synthetic biomimetic complexes have been employed providing further details into the chemistry at the metal center. While organic substrate oxidation chemistry has been studied, the reactivity of highvalent, nonheme metalloenzyme intermediates and synthetic complexes with hydrogen peroxide (H2O2) has not been reported. This potential reaction could be of interest in biological systems due to the fact that analogous high-valent oxoiron(IV) species are the proposed reactive intermediate in decomposing H2O2 in the heme containing catalase enzymes. This potential reactivity, in combination with the dual roles of H2O2 as both a signaling molecule and potentially damaging oxidant, could provide both detrimental and beneficial functions to biological systems. Our current studies have shown that the oxo moiety of synthetic high-valent nonheme intermediates can directly react with H2O2. Insight into how various ligands affect the reactivity of nonheme, high-valent oxoiron(IV) complexes with H2O2 will be discussed.
Redox and Spin State Tuning in Iron Triaza Macrocyclic Complexes

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Banerjee, Atanu; Oakland University, Chemistry
Panda, Manashi; Oakland University, Chemistry
Stjepanovic, Slavica; Oakland University, Chemistry
Brennessel, William; University of Rochester, Chemistry
Loloee, Reza; Michigan State University, Physics and Astronomy
Chavez, Ferman; Oakland University, Chemistry

Metal complexes containing triazamacrocyclic ligands have been extensively studied due to their biologically relevant structures. One of the most studied members of this class of ligands is 1,4,7-triazacyclononane (tacn) due to the stability derived from three five-membered chelate rings. In this study, we examine the influence of expanding the ring size by one CH2 group (1,4,7-triazacyclodecane, tacd) and two CH2 groups (1,4,8-triazacycloundecane, tacud) on the magnetic and electrochemical properties of FeII bis-chelates. Iron(II) complexes of tacn, tacd, and tacud have been synthesized and fully characterized. Redox studies on these complexes reveal [Fe(tacud)2](OTf)2 is a stronger oxidant than [Fe(tacn)2](OTf)2 and [Fe(tacd)2](OTf)2. In addition, magnetic studies show that [Fe(tacud)2](OTf)2 is a purely high spin complex under ambient conditions whereas [Fe(tacn)2](OTf)2 and [Fe(tacd)2](OTf)2 exhibit spin equilibrium.

Nanoparticle Epitaxy using Self Assembled Nanoparticle Monolayers as a Substrate

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Epitaxy is commonly used in semiconductor fabrication and refers to a layer by layer process in which a crystalline film is grown on a substrate. A unique aspect of epitaxial growth is that the film's crystalline structure is controlled by the lattice parameters of the underlying substrate. Epitaxial growth has been extensively studied in atomic systems from amorphous films. Herein, we have extended this process as a method to assemble nanoparticle heterostructures. Textured monolayers of self assembled nanoparticles provide a suitable substrate for the formation of complex nanoparticle interfaces via an epitaxial growth relationship. By controlling the size ratio of the nanocrystals in substrate and epitaxy layers, different surface reconstructions are possible. The use of similar sized nanoparticles resulted in an epitaxial layer retaining the hexagonal structure of the substrate layer, however, nanoparticles with a diameter approximately half of those in the substrate layer resulted in an AB2 structure. In addition, the effect of the Hamaker constant on the interparticle interactions in the epitaxy layer was explored by changing the composition of the nanoparticles in the epitaxy layer. Varying the strength of the Hamaker constant influenced the mode of epitaxial growth observed. The extension of epitaxial growth to self-assembled nanoparticle systems provides not only a model system with precise tunability of the lattice parameters through control of the nanoparticle size, but also potential in the design of functional materials through the proper choice of technologically important nanoparticles in the different layers.
The Effect of Side-chain Length on Guest Binding and Enantiomeric Selectivity of Gd-based Metallacrowns

Joseph Grant and Vincent L. Pecoraro
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Molecular hosts that encapsulate guest molecules have applications in catalysis, separations, and stimuli responsive materials. Metallacrowns (MCs) are molecular hosts composed of a central metal connecting ligand side-chains. The ligand side-chains arrange to form a hydrophobic “pocket” that has been shown to encapsulate guest molecules. In this study, Gd-MCs with various side-chains and guest molecules were studied. The hydrophobic cavity influences guest recognition and enantioselectivity. Guest binding was measured with a cyclic voltammetry competitive binding assay using ferrocene carboxylate (FcC) as a redox probe. The experiments presented here used ligands with phenyl side-chains containing 0, 1, and 2 methylene spacers, labeled here as L-pgHA, L-pheHA and L-hpheHA, respectively. From this data, Gd-hpheHA MC has shown to have the greatest bond affinity to FcC with a binding constant of 12000 ± 700 (M⁻¹). Gd-pgHA and Gd-pheHA MCs had significantly lower binding constants of 5000 ± 400 and 4500 ± 700 (M⁻¹), respectively. The discrepancy between these binding constants is likely because Gd-hpheHA MC can completely encapsulate the FcC molecule, while Gd-pgHA and Gd-pheHA MCs cannot. The smaller side-chains of Gd-pgHA and Gd-pheHA MCs prevent a proper hydrophobic cavity from forming. When titrating a different guest molecule, sodium benzoate, a similar trend was noticed with Gd-hpheHA MC displaying a significantly greater binding affinity to sodium benzoate than the other MCs. Enantiomeric selectivity between R/S-mandelate could also be seen with Gd-pgHA and Gd-hpheHA MCs. In both MCs, binding affinity to S-mandelate was two times as great as the binding affinity to R-mandelate. Given the enhancement in selectivity and chiral recognition through changes in the hydrophobic cavity, we are exploring different side-chains that could lead to more selective guest binding. These highly selective hosts could be immobilized on solid phases for use in large-scale separations processes.

Characterization and Optimization of Palladium Nanoparticles on Porous Polycarbonate Membranes as a Catalyst for the Suzuki Coupling Reaction

Lyndsey Reynolds and Kevin Metz
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The Suzuki coupling reaction produces carbon-carbon bonds between substituted phenyls in aqueous media and is beneficial for many reasons. While it has made significant impacts in the synthetic chemistry and chemical industries, it still has some shortcomings. Most notable are the need to remove palladium from the products and needing to clean palladium out of the reaction vessels at the plant scale. This research focuses on resolving these issues by developing and optimizing a new flow through reactor method utilizing palladium nanoparticles on membranes. The optimization of the method can be scaled to the industrial level and will be more efficient than current methods for running the Suzuki reaction. This method involves a flow through reactor pushing the reactants through the membrane, exposing them to palladium nanoparticles, while not directly mixing the nanoparticles in the solution. To date we have found that there is no statistical difference in percent yield from membranes with different pore sizes and from membranes that are in the plating solution for different amounts of time. However, we did find statistical differences in rate of reaction and temperature.
**Studies of Metal Binding to Riboflavin Binding Protein: Ruling out the Adventitious**

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Riboflavin binding protein (RBP) is being studied as a possible transport and storage system for Cu ion in avian embryo. Preliminary studies performed on eggs deprived of Riboflavin (Rf) show that RBP is still present in the eggs, suggesting an additional role beyond active transport of Rf into the egg. Hens fed excess Cu do not lay eggs containing excess Cu, implying that Cu intake is highly regulated by system or systems unknown. It has been previously shown in the Smith/Benore laboratories that RBP binds Cu in a one-to-one stoichiometry *in vitro*. Studies on freshly purified protein have shown only trace amounts of copper. Currently, RBP’s role in Cu storage is being studied via determination of its binding constant and competition with other metals such as zinc in order to rule out adventitious binding of the metal ion. Since the bound copper exists in a mixture of oxidation states, it has also become critical to develop appropriate conditions to keep Cu in one oxidation state. This poster will present our progress towards these goals.

**Preparation and Characterization of Tunneled and Layered Structures for Potential Iron Based Cathode Materials**

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New mixed-valent layered lithium iron oxides, \(\alpha\)- and \(\beta\)-LiFe\(_2\)O\(_3\), as well as a new LiFeTiO\(_4\) polymorph with a tunnel structure were synthesized by multistep soft-chemistry route. The \(\alpha\)- and \(\beta\)-LiFe\(_2\)O\(_3\) phases were prepared from corresponded NaFe\(_2\)O\(_3\) by low temperature exchange of Li\(^+\) for Na\(^+\). Delicate control of oxygen pressure is required for preparation of NaFe\(_2\)O\(_3\) due to mixed valent character of phases and easy polymorphs transformations. Partial oxygen pressure ranges of stability NaFe\(_2\)O\(_3\) polymorphs were established. We have synthesized a new LiFeTiO\(_4\) polymorph with CaFe\(_2\)O\(_4\)-type structure by low temperature exchange reaction from NaFeTiO\(_4\). One can relate CaFe\(_2\)O\(_4\) to NaFeTiO\(_4\) by double aliovalent (different valent) substitutions: Ti\(^{4+}\) for Fe\(^{3+}\) and, to maintain the charge balance, Na\(^+\) for Ca\(^{2+}\). LiFeTiO\(_4\) has a tunnel structure built up by (Fe/Ti)O\(_6\) octahedra that form double edge-sharing chains. The edge-sharing Fe\(_2\)O\(_{10}\) dioctahedra also vertex share to other Fe\(_2\)O\(_{10}\) dioctahedra, a connectivity that gives rise to the “double rutile” chain: the lithium ions are located in a single tunnel surrounded by four chains.
Principal component analysis (PCA) for chemometric study of 2-D spectroscopic data is commonly employed in the identification and quantification of materials and biological specimens. PCA is powerful in that it can reveal critical regions within spectra that can be used to distinguish between samples. These regions of interest may occur as single wavelengths or combinations of wavelengths. However, analyses that utilize PCA in this manner do not fully exploit the data present in a spectrum because samples without markedly different spectra or clear identifying peaks can be difficult to discern. Most analyses are also limited by using PCA in conjunction with measures of hyperdimensional distance to differentiate between distinct chemical entities rather than mixtures of compounds.

This study analyzes 2-D FT-IR microspectroscopic data taken from the abdominal aortas of healthy mice and those affected by abdominal aortic aneurysms (AAAs). AAAs are a dilation of the abdominal aorta to above 1.5 times its normal diameter, a condition that may lead to vessel rupture and death. Studies have indicated that shifts in the ratios of structural proteins in the aorta are responsible for the development of AAAs. In this analysis, PCA was performed on data sets composed of single IR spectra for each 6.25 μm × 6.25 μm pixel in a tissue slice. To determine relative chemical similarities, Mahalanobis distances were calculated from the PC space determined from the raw spectral data and a reference spectrum of interest. 2-D images were generated using MATLAB® to display these similarities in a false-color gradient. This technique is very useful in the examination of samples with continuous distributions of compounds. Furthermore, the comparison of different spectra in PC space—rather than based on wavelengths of interest identified through PCA—incorporates the majority of the variance in spectral data in the event that there are no critical regions discernible by PCA or the human eye.

The purpose of this work was to design a lab for students to learn the electrochemistry and associated calculations involved in commercial blood glucose monitoring. Glucose monitors use a disposable testing strip that employs glucose oxidase and hexamine ruthenium (III) chloride. These compounds act, respectively, to oxidize glucose and to shuttle electrons to an electrical circuit. Commercial, screen printed glucose electrodes were coupled to an FS522 MicroLab data acquisition interface for data collection. Through the analytical technique of chronoamperometry, the electron transfer between glucose and the electrode was measured. These data were analyzed using the Cottrell equation and provided useful data on the amount of glucose in a solution.
The Development and Analysis of Ionochromic Azo Dyes for Aqueous Halide Detection

Heather Robison, Noel M. Paul, J. Clay Harris
The Ohio State University

Interactions of halide ions in aqueous solution with organic dyes will be exploited to determine concentration based on color change utilizing spectrophotometric methods. A survey is being conducted to determine if commercially-available organic dyes have interactions with chloride, bromide, and/or iodide ions independent of pH change. Findings have included promising dye interactions in particular with sudan black B and janus green B. These molecular motifs will be incorporated into more sophisticated dyes through organic synthesis in search of an enhanced interaction with the halides. In one such synthetic route, a desired result is for the molecule to behave with the solution phase similar to a bilayer. The dye phases may exhibit improved indicator properties as the hydrophobic zone may help to exclude water and improve specific non-covalent interaction between a halide and a charged dye structure to shift the wavelength of absorption an appreciable amount. By developing an indicator that creates a favorable interaction with each halide ion in water, halide concentrations could be measured with extreme accuracy and precision at a much lower cost. Ultimately, measurements could be taken in various environments, specifically living cells to measure halide gradients.

The Influence of Aromatic Amines on the Spectroscopic Properties of 1,10-Phenanthroline

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The B-ring of 1,10-phenanthroline was functionalized by introducing different aromatic amines such as aniline, 1-naphthylamine, and 1,5-diaminonaphthalene via nucleophilic addition to 1,10-phenanthroline 5,6-epoxide. The properties of the resulting amino alcohol derivatives were examined using UV and fluorescence spectroscopy. In addition, their interaction with DCP was studied by monitoring changes in absorbance.
Synthesis of Betulinic Acid Analogues as Potential Anti-Arthritic Agents

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Rheumatoid Arthritis (RA) has no available cure. The drugs used for RA treatment only deal with regulation and management of pain. The triterpenoid natural product betulinic acid has been shown to possess anti-melanoma, anti-inflammatory properties and also the potential to induce apoptosis. Studies have indicated that betulinic acid is able to induce apoptosis in apoptosis-resistant synovial cells implicated in arthritis, and is therefore a potential agent for RA treatment. Analogues of betulinic acid were synthesized to determine the structure-activity relationship (SAR) requirements for its apoptosis-inducing properties as well as to develop more potent analogues. The synthesis of these analogues will be presented.

1,10-Phenanthroline Derivatives as Potential Organophosphate Sensors

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The goal of this project was to modify the substituents in the 5- and 6-position of 1,10-phenanthroline and to study whether hazardous organophosphates could be detected. The molecules were prepared via nucleophilic addition of different aromatic amines to 1,10-phenanthroline-5,6-epoxide which served as key intermediate. Fluorescence measurements were conducted with diethyl chlorophosphate (DCP). A molecule derived from 2-aminopyridine displayed interesting changes in absorption during the titration of the analyte.
Development of Isothermal Amplification of DNA

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Quadruplex priming amplification (QPA) is a new method that has been shown to facilitate nucleic acid amplification and real-time nucleic acid quantification. The method relies on specifically designed 13-nucleotide primers (GGGTGGGTGGGTG), which, after adding two guanines, are capable of spontaneously dissociating from target sites and forming a DNA quadruplex. The quadruplex is characterized by significantly more favorable thermodynamics than the corresponding DNA duplexes. As a result, target sequences are accessible for the next round of priming, and DNA amplification proceeds under isothermal conditions with improved product yield. However, under the current design, QPA is not truly isothermal and requires extra steps to incorporate the appropriate primer binding site sequences within nucleic acid templates. Our ultimate goal is to design a truly isothermal amplification/detection assay. For this purpose, we are using a 14-nucleotide long primer (GGGTGGGTGTTGGTGG), which, upon addition of one guanine, is able to self-dissociate from target DNA. We will report on our UV absorption and fluorescence studies of GGGTGGGTGTTGGTGGG and GGGTGGGTGTTGGTGG sequences, which established the most favorable experimental conditions for truly isothermal QPA. The use of nonspecific priming confers the added advantage that the target nucleic acid sequence does not need to be known and eliminates the need for temperature cycling in nucleic acid amplification and real-time quantification.

Peracylation of Pentaerythritol

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The purpose of manipulating the peracylated product that is synthesized from pentaerythritol is mainly to see if all four alcohol groups are able to be replaced with four acyl groups—and then analyze the product to see if complete esterification took place. Analysis with chromatography, recrystallization and NMR is very difficult with the beginning compound due to the very polar nature of pentaerythritol. The purpose then was to make an ester compound out of a polyol compound. Complete peracylation of a polyol compound is rare and that is why the very important method of imidazole catalysis was employed for this experiment. This was an advantage specifically to this experiment because imidazole is especially good at attacking the carbonyl group and then being displaced—this aided tremendously in converting all four alcohol moieties. The method by which manipulation of pentaerythritol took place was through substitution and esterification (also called peracylation). The beginning compound was mixed with imidazole and acetic anhydride, heated in a microwave oven, and then through Buchner filtration and washing was purified to remove the catalyst and other impurities. Results were very clear in showing that the alcohol was completely esterified. This was confirmed through TLC, $^{13}$C and $^1$H NMR and FTIR spectrosopies. Even with an FTIR reading that was very clear in showing that esterification took place the average melting point had a range of almost 14°C which is evidence for low purity, in contrast to the evidence for high purity resulting from FTIR and NMR spectroscopy.
As bacteria grow more and more resistant to current antibiotics, a significant amount of diseases may put the whole human society in danger due to the lack of treatment. Research and production of antibiotics with new moieties is needed. Varying substituents at the C-3 position on cephalosporin cores has been an important strategy in developing new and effective antibiotics. The nucleophiles commonly used generally have heteroatoms that serve as the nucleophilic site. This project will use carbon nucleophiles which appears to be surprising unexploited in the literature. This research project is to associate a nucleophile to cefotaxime to form molecules containing electron withdrawing groups. Diethyl malonate is used as one of the nucleophiles, and the procedure of the reaction was adopted from the malonic ester synthesis. Diethyl malonate was the first candidate because malonic ester synthesis is a well-established and relatively straightforward reaction, making this approach promising for pharmaceutical applications.

1,10-Phenanthroline is a well-known ligand for supramolecular chemistry. For example, we found that the introduction of 2-aminopyridine in the 6-position caused a change in absorption when it was titrated with diethyl chlorophosphate. In order to identify the binding mechanism we investigated the role of the diimino moiety of 1,10-phenanthroline through comparison with related phenanthrene derivatives.
Electrocatalytic Upgrading of Biomass Pyrolysis Oils to Hydrocarbon Fuel

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The high specific energy, chemical stability, and relatively low toxicity of hydrocarbons make them ideal as transportation fuels. But as their source—fossil petroleum—grows rarer and more expensive, and the impacts of rising atmospheric CO₂ starkly emerge, world chemical and energy industries must shift to a renewable, carbon-neutral basis: Biomass. This large-scale challenge is ultimately one of economies—of money, energy, and carbon—and the chemical pathways needed to practically enable the shift.

Plants capture solar energy and carbon, so huge investments of genius, equipment, money and time are focused on converting biomass to liquid fuels such as ethanol, biodiesel, butanol, etc. This approach cannot address the problem’s scale, for three reasons (1) Insufficient energy and carbon: in the US, the energy and carbon contents of petroleum used exceed by factors of ~2 and ~1.3 the analogous quantities in all available annually harvestable non-food biomass. (2) Inefficient energy capture and (3) Low specific energy: plants only store ca. 1% of the sun’s energy in chemical form, and ton for ton, biomass has only ~⅓ the energy of hydrocarbons (15 MJ/kg vs. 45 MJ/kg). Thus, as they concentrate energy from inadequate, dilute energy and carbon pools, today’s fuel-making bioprocesses discard ⅓ – ½ of input carbon.

An alternative two-step approach uses (1) biomass fast pyrolysis (BFP) to liquefy biomass. The resulting “bio-oil”, a viscous, corrosive mix of oxygenated organics, is like biomass in specific energy. Incompatible with classical liquid fuels, it requires (2) upgrading by dehydration, deoxygenation, and hydrogenation to raise energy content and maximize carbon retention. These hydrocarbon-forming reductions employ electricity, the energy form from man-made solar energy capture technologies that are more efficient than plants (e.g. ~10% for photovoltaics). Thus, our studies seek robust, scalable electrocatalytic hydrogenations (ECH).

This work focuses on ECH of lignin–derived aromatics found in bio-oil. Traditionally, hydrogenation of aromatic bonds requires energy demanding conditions and expensive catalysts such as Pt or Pd. Mild ECH reactions have been reported, but cost remains an obstacle to process scaleup. Fortunately, Raney-Nickel (a high surface area form of nickel) has the potential to be compatible with the precious metal in aromatic ECH, and its effect can be improved by adding cationic surfactants, aka surface active reagents. With surfactant, the ECH efficiency of bio-oil derivatives improves significantly. With these exciting findings, we continue to optimize the conditions in which unsaturated double bonds can be hydrogenated efficiently.

Interaction Pyridine Derivative Dyes as Halide Selective Indicators in an Aqueous Solution

Jason Lee, Kurt Justus, Dr. Noel M. Paul, Dr. J. Clay Harris
The Ohio State University
**22A**

**Resonance and the Silicon-Carbon Double Bond**

*Greg Kortman, Randy Winchester*  
*Grand Valley State University*

The allyl anion is a primary carbanion attached to a carbon-carbon double bond. It has fundamental significance, because it is the smallest organic molecule that displays resonance between two possible Lewis structures which gives the molecule added stability. The allyl anion is also of practical interest because of its similarity to the intermediate in anionic butadiene polymerization, which is important in the production of rubber. One measure of the extra stability due to resonance for the allyl anion is its rotational barrier, which has been found to be 10.7 kcal/mol for allyllithium.

The silaallyl anion is what is formed if one replaces a carbon atom of the allyl anion with a silicon atom. Like the allyl anion, the silaallyl anion has both practical and theoretical significance. Practically, the silaallyl anion could be useful as a ligand on transition metals or as an intermediate in the formation of new polymers. Once the silaallyl anion has been synthesized the rotational barrier can be measured in a manner similar to that for the allyl anion, which will be useful for determining the significance of the resonance structure of the silaallyl anion.

The steps that lead to the silaallyl anion have been optimized and a convenient method for modifying the substituents at silicon has been developed. Previously chlorodiphenyl(vinyl)silane was reacted with lithium which should form the anion through a radical pathway, but the diphenyl system proved to not be sterically hindered enough to inhibit polymerization so larger protecting groups needed to be explored. We are investigating the use of the chlorodimesitylvinylic silane as one route to the silaallyl anion. A second route we have studied involved synthesizing 1,1,3,3,3-hexamethyl-2-vinyltrisilane and then studying its reaction with tert-butylithium. We observed a color change which is indicative of the formation of the silaallyl anion, but because prior steps lead to products that are difficult to isolate, we did not have enough anion to fully characterize it. The 1,3-di-tertbutyl-1,1,3,3-tetramethyl-2-vinyltrisilane system is being synthesized which should solve the issues involved in the synthesis of 1,1,3,3,3-hexamethyl-2-vinyltrisilane and give us more of the product anion to study. Currently methods of deprotonation of 1,1,3,3,3-hexamethyl-2-vinyltrisilane and trapping of the anion are being explored.

**22B**

**Combinatorial Chemistry: Multiple Product Transesterification**

*Kyle Thompson, Dr. Bruce Baldwin*  
*Spring Arbor University*

Transesterification is a process through which an ester group can be moved from one molecule to another, such as in biodiesel synthesis. The biodiesel transesterification process is a simple and relatively green way to make an alternative fuel source using only a vegetable oil, an alcohol solvent, and a hydroxide salt. As a model for green transesterification, the biodiesel procedure was modified into a short-chain ester combinatorial synthesis. Combinatorial synthesis is a method in which multiple desired products are created in the same experiment mixture. In this setup, multiple short-chain alcohols are put into a mixture with one or more triglycerides along with potassium hydroxide to act as a catalyst. After applying heat and refluxing the mixture for the required time, the products were filtered using a condensation distillation glassware apparatus. The products were then analyzed using FTIR and gas chromatography. The products were then compared against commercially produced compounds to determine the identity and purity of the chemicals in the sample. The experiment is designed to be as green as possible. The alcohols are both reagents and solvents, so no extra or potentially harmful chemicals are needed. There is a small amount of waste produced from the experiment, but it is relatively nontoxic. Through the variation of reagents used, this experiment can teach students about modifying a general method to maximize their results and how to analyze products so as to identify multiple compounds in a single mixture.
Interactions of Pyridine Dye Derivatives as Halide Selective Indicators in an Aqueous Solution

Kurt Justus, J. Clay Harris, and Noel M. Paul
The Ohio State University

Several commercially available dyes have been tested in an attempt to verify a halide selective indicator in various solvents but have yet to show much efficacy in an aqueous solution. Currently, studies are taking place of various simple dyes synthesized containing a central azo functional group and a measurement of the molecule's selectivity for particular halides. Primarily the dyes synthesized thus far have included benzoic acid groups, a domain group, and a functional group. In this study, an attempt to synthesize molecules replacing acidic substituted anilines with pyridyls was studied as well as recorded measurements of any halide selective ability. The results have helped to further develop an understanding of azo-dye anion indicators as well as give insight to pyridyl derivatives and the reactivity of those compounds. The long term goal of this work is to create a molecule with wide variability in halide selectivity, is rather inexpensive and simplistic in its synthesis, and water soluble. The dye molecules could ideally be used in water treatment systems or even on the biomolecular scale to monitor anion activity/movement.

Synthesis of Glowing Chalcone from 1,4-diacetyl benzene

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Spring Arbor University

The purpose of this experiment was to synthesize glowing chalcone from 1,4-diacetyl benzene and 4-methoxy cinnamaldehyde and obtain a pure product through column chromatography. The experiment was based upon the aldol condensation. Several column chromatography procedures were implemented in this experiment in order to separate the impure product and to increase the purity of the desired product. The product of this experiment had a lower IR wavelength number than the starting materials, indicating shift of the carbonyl and an increase in conjugation. The product also fluoresced under a UV lamp because of the structure's push-pull effect caused by the methoxy group (the pusher) and the carbonyl group (the acceptor). The melting point range of the product had a wide range, indicating impurity in the product. Moreover, the IR peaks of the product had some peaks similar to those detected in the starting materials, implying that some unreacted 1,4-diacetyl benzene (starting material) co-migrated with the sample in chromatography. On the other hand, the IR of the product after chromatography had more resolved peaks than the product before chromatography, indicating some separation. In addition, there were no similar peaks between the product and the starting material 4-methoxy cinnamaldehyde, meaning this starting material was well-reacted. In conclusion, this experiment did not result in the production of a pure chalcone product from the reaction of 1,4-diacetyl benzene with 4-methoxy cinnamaldehyde. This may be because a different method than column chromatography is needed to obtain a pure product.
24A

Modification of the Procedure for the Growth and Purification of Cytochrome c Peroxidase (CcP)

J. Travis, G. MacLean, C. DiCarlo
Grand Valley State University

The required modifications for the growth and purification method of D34K, D79K, and E118K novel protein mutations were determined. The mutation caused changes to the growth ability of the proteins which resulted in a decreased amount of hemin needed. The hemin amount was decreased because extra hemin could disrupt the purification process and destroy the protein. Also, the amino acid’s interactions with the solutions in the environment were altered due to the mutation’s locations on the surface of the protein and the mutation changing the amino acid from a polar acidic to a polar basic. The change from acidic to basic caused the mutated protein to elute out with a lower concentrated mobile phase compared to the wild-type CcP. Crystallization of the D34K and D79K was achieved through the use of ion exchange chromatography, size exclusion chromatography, and dialysis.

24B

Reductive Cleavage of N-O Bonds in Weinreb Amides by NaSG

Max Braun, Brittany O’Brien, Ned Jackson, James Dye, Bryan Dunyak
Michigan State University

Sodium in silica gel performs a clean reductive cleavage of N-methoxy-N-methyl-benzamide and possibly other Weinreb amides. The room-temperature stable nature of this reagent provides a safe, simple, alternative to the usual metal based reductive cleavage.

\[
\begin{align*}
\text{N-methoxy-N-methyl benzamide} & \quad \xrightarrow{5 \text{ equiv. NaSG}} \quad \text{N-methyl benzamide} \\
& \quad \xrightarrow{H^+} 
\end{align*}
\]
Boronate Urea Catalyzed Reactions of Strained Rings

Victoria Garza, Sonia So, Tyler Auvil, Anita Mattson
The Ohio State University

Reactions catalyzed by small organic molecules through non-covalent interactions are emerging as powerful tools for the synthesis of valuable target molecules. Specifically, hydrogen bond donors (HBDs) are useful non-covalent catalysts able to interact with a variety of functional groups and operate in a number of transformations. Boronate ureas have been identified as a new class of HBDs with enhanced reactivity due to the strategic placement of an internal Lewis acid. Specifically, in comparison to conventional ureas, boronate ureas benefit from lower catalyst loadings, reduced reaction times and access to unique reactivity patterns. To this end, we have discovered boronate ureas operate as catalysts for the activation of nitrocyclopropanes in nucleophilic ring-opening reactions giving rise to valuable nitro ester building blocks in good yield. Details behind the development of boronate urea activation of nitrocyclopropanes, including mechanistic investigations and applications toward the synthesis of bioactive targets, will be presented.

Synthesis and Gelation Test of Cystine Derivatives for TATP Detection

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University of Michigan – Ann Arbor

Triacetone triperoxide (TATP) is difficult to detect using conventional explosives detection methods. Yet it is easy to synthesize by over-the-counter ingredients, making detection a high priority. Our research is focused on developing sensors for TATP using the solution-to-gel phase transition. TATP is known to decompose into hydrogen peroxide (H$_2$O$_2$) when treated with acid. Thus, we developed a sensor that responds to H$_2$O$_2$. The sensor utilizes thiol oxidation to generate the gelator molecule (disulfide) and trigger gelation. Our preliminary results showed that gelation can be triggered by TATP. To increase sensitivity, we have been developing gelators with lower critical gel concentrations. Specifically, the para position on the naphthyl group was modified to influence the intermolecular interactions and packing structure. Several new gelator molecules were discovered among these derivatives. Our current efforts are focused on alternative design strategies, including adding amino acids between the reactive thiol and unreactive naphthyl groups.
Thinking about going to grad school?

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