

UNDERGRADUATE RESEARCH POSTER SESSION

The Lehigh Valley Section of The American Chemical Society

Moravian College

April 22, 2008

1. EVALUATION OF THE ANALYSIS OF DIAMONDROID COMPOUNDS IN KEROSENE RESIDUES BY GAS CHROMATOGRAPHY/MASS SPECTROMETRY FOR USE IN FIRE DEBRIS ANALYSIS

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Forensic Scientists often play a critical role during the investigation of suspicious fires by analyzing fire debris samples for accelerant residues. However, the detection of ignitable liquid residues can be a difficult process. It has recently been found in the environmental field that diamondoid compounds can be detected in heavy range petroleum distillates and can be used to determine a specific ion pattern for petroleum products. Diamondoids are rigid, three dimensionally fused cyclohexyl alkanes that are naturally found in crude oil. They have a high thermal stability and are not easily affected by refining, weathering, or biodegradation making them ideal analytes for fire debris analysis. By using gas chromatography/mass spectrometry (GC/MS), molecular ion fingerprints for diamondoids can be developed and used to identify these fuels in fire debris.

Using passive and heated static headspace, adamantanes were successfully isolated and identified by GC/MS from liquid kerosene and kerosene residue samples.

2. INVESTIGATION OF THE EFFECT THAT DIFFERENT DRYING METHODS HAVE ON THE MECHANISM OF THEOPHYLLINE RELEASE FROM MICROCRYSTALLINE CELLULOSE BEADS.

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Samples of microcrystalline cellulose, MCC, and 10% theophylline were granulated, extruded and marumerized into wet sustained release beads. These wet beads were then exposed to several different drying methods including: freeze-drying, convection oven drying, and exposure to four different humidity conditions. The rate of theophylline release from the MCC bead systems was measured by dissolution methods using 0.01 molar hydrochloric acid as the dissolution media or solvent. The control for this experiment was the convection oven dried beads. The results observed, based on these dissolution studies, suggest that the rate of theophylline release from each MCC dried bead system, either increases, decreases or follows the same release rate as the control sample. Which further suggests that the rate of release of theophylline from each MCC sample depends on the drying method used to dry the wet bead systems.

3. DETERMINATION OF SELENIUM IN RAT TISSUE AND RAT DIET SAMPLES

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Selenium has been shown to inhibit heavy metal toxicity in mammals, with evidence that it can decrease oxidative brain damage in Fisher 344 rats with a lesion model for Parkinson's disease. Tissue samples were harvested from rats fed either a control diet or a selenium-enriched diet. This study used Graphite Furnace Atomic Absorption Spectroscopy (GFAAS) to determine if low levels of selenium in complex tissue and food samples could be detected, if selenium tissue levels were statistically different in the two different rat groups, and if selenium measurements were accurate and reproducible. Samples were prepared by microwave digestion in nitric acid and then GFAAS was used to determine levels of selenium. For rat food samples, issues of sampling and accuracy of selenium content were investigated. Results indicate that the average amount of selenium for food samples may be significantly less than reported by the manufacturer. Tissues results were inconclusive.

4. THE INVESTIGATION OF GAMMA-HYDROXYBUTYRATE AND RELATED COMPOUNDS AS POSSIBLE INTERFERENTS IN THE ANALYSIS OF BREATH ALCOHOL UTILIZING THE ALCOTEST 7110MK III-C

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The Dräger Alcotest 7110MK III-C is an evidentiary breath-alcohol testing instrument which uses both infrared spectroscopic and electrochemical detection. The instrument has been available to law enforcement for many years; however, this instrument has just recently been released to institutions other than law enforcement. Although some testing for interferents has been performed using this instrument, the effects of gamma-hydroxybutyrate (GHB), its precursors, and analogs, have not been tested on the Alcotest 7110MK III-C. GHB, gamma-butyrolactone (GBL), and butanediols are commonly abused drugs that are often taken simultaneously with alcohol. This study determined that the following substances showed no interference with the determination of breath alcohol concentration: GBL, 1,2-butanediol, 1,3-butanediol, 1,4-butanediol, 2,3-butanediol and GHB. Concentrations tested of GHB and related compounds ranged from 0.23 mg/mL to 1.12 mg/mL in both water and ethanol.

5. INVESTIGATION OF THE EFFECT THAT DIFFERENT DRYING METHODS HAVE ON THE MECHANISM OF ACETAMINOPHEN RELEASE FROM MICROCRYSTALLINE CELLULOSE BEADS.

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Samples of microcrystalline cellulose, MCC, and 10 % acetaminophen were granulated, extruded and marumerized into wet sustained release beads. These wet beads were then exposed to several different drying methods including: freeze-drying, convection oven drying, and exposure to four different humidity conditions. The rate of acetaminophen release from the MCC bead system was measured by dissolution methods using distilled water, 0.01 molar hydrochloric acid, pH 2.0 or sodium phosphate buffer, pH 8.0 as the solvent systems. The control for this experiment was the convection oven dried beads. The results observed, based on these dissolution studies, suggest that the rate of acetaminophen release from each MCC dried bead system; either increases, decreases, or follows the same release rate as the control sample. Which further suggests that the rate of release of acetaminophen from each MCC sample depends on the drying method used to dry the wet bead system.

6. SIGNIFICANCE OF SONIFICATION VARIABLES IN MINIEMULSION PREPARATION

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Emulsion polymers have many uses, from paints and coatings to adhesives. Some monomers can not undergo conventional emulsion polymerization due to high water insolubility; miniemulsion polymerization is an alternative. Miniemulsions are stable dispersions of submicron droplets often prepared with a sonifier. There are a vast number of variables inherent in sonification; their effect on miniemulsion droplet size and stability is unknown. To determine which variables are most significant, an experimental program using Plackett-Burman design was conducted. Miniemulsions of identical recipe were prepared while adjusting the sonification variables according to the experimental design matrix. The effect of each variable was determined by measuring the droplet size and amount of oil that separated from the emulsion, then calculating the variance and significance of the effect. It was found that duration and sonifier power level are most significant, while sample and container size, mixing, and temperature control surprisingly had little effect.

7. PREPARATION OF IONIC LIQUIDS AND THEIR USE IN THE SYNTHESIS OF POLYAMINE ANALOG REACTIONS

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This investigation will involve the preparation of several ionic liquids containing the 1-hexyl-3-methylimidazolium cation coupled to various anion systems. These ionic liquids can be substituted for typical organic solvents and used in the substitution reactions of spermidine to produce several spermidine analogs. There are many advantages for using these ionic liquids over organic solvents in synthesis reactions. Ionic liquids are recyclable, they can stabilize intermediates better than traditional solvents and the product yield is much higher. The ionic liquids can also be used for synthesis at lower temperatures and are a less toxic alternative to typical organic solvents.

8. A STUDY OF IONIC LIQUIDS FOR APPLICATIONS IN THE CONTINUOUS SEPARATION OF BUTANOL FROM FERMENTATION MEDIA

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The annual consumption of gasoline in the United States is only expected to increase. The amount of oil found is steadily decreasing and the price continues to rise. Due to this, many countries and companies are exploring alternatives for fossil fuels. One main alternative, being put in place for automobile use, is ethanol. Butanol however, has many advantages over ethanol. Currently butanol is produced using petroleum feedstocks, but recently attention has been focused on fermentation derived butanol.

Improvements to the butanol separation process could lead to cost-effective biologically derived butanol. A proposed method would utilize liquid-liquid extraction. The solvent selected being a hydrophobic ionic liquid that is able to dissolve large amounts of butanol. This research investigates the choice of ionic liquid based on phase behavior between several ionic liquids, butanol, and water. Additionally, other pertinent information about the chosen ionic liquid (Cyphos 102) was investigated.

9. ANILINE TRIMERS WITH MULTIPLE TERMINAL GROUP SUBSTITUTIONS AND CROSS LINKING OF SELECTED PRODUCTS

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Polyaniline has been studied by many groups because of its potential as an anti-rusting agent and its conductive properties. The polymer itself is difficult to work with because of its low yield when synthesized and a distinct lack of solubility. Small units of the polymer known as trimers go into solution readily in many solvents and are easily synthesized in sizable amounts. Eight trimers were synthesized each with different terminal groups. To verify the structures IR and NMR was used. The anthranilic and 2-hydroxy trimers both had prominent peaks around 1000 cm^{-1} , 1500 cm^{-1} , and stretches from $3000\text{-}3400\text{ cm}^{-1}$. These two trimers were cross linked with Co^{+2} , Zn^{+2} , Ni^{+2} , Fe^{+2} , and VO_2^{+2} at their terminal hydroxyl/ carboxylic acid and NH_2 groups. Each of the cross linked products were confirmed using IR with shifts in the prominent peaks and a virtual elimination of the $3000\text{-}3400\text{ cm}^{-1}$ stretch in each.

10. LASER SYNTHESIS OF LINEAR POLYYNES

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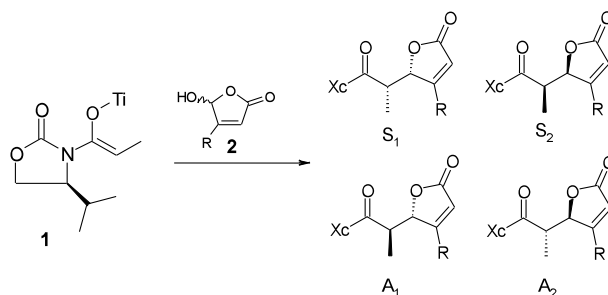
The laser ablation of graphite particles suspended in solution was performed using the second harmonic of an Nd:YAG laser (532 nm). Product analysis using Gas Chromatography – Mass Spectrometry revealed the formation of C_nH_2 polyynes ($n = 4, 6, 8, \text{ and } 10$). An analysis was done to compare the usage of different solvents with varying graphite concentrations, as well as alternate carbon sources. From the results, it was determined that simple alcohols produce the highest yield of desired product. The halogenated solvents provided insight to the hydrogen capping of the polyyne, indicating that the hydrogen capping results from the solvent. The presence of odd-numbered carbon chains provided insight to the mechanism of the formation of the polyyne carbon chain.

11. THE ADDITION OF CHIRAL ENOLATES TO ACHIRAL γ -HYDROXYBUTENOLIDES

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We employed the titanium enolate of (S)-3-(1-oxopropyl)-4-(1-methylethyl)-2-oxazolidinone (also known as Evans' oxazolidinone), **1**, in designing a stereoselective synthesis of optically γ -lactones by means of an asymmetric aldol reaction with representative gamma-hydroxybutenolides, **2** (where R = Ph, ⁱPr, Me and H). The reactions gave good yields (74-94%) of a mix of γ -lactones of which the S_2 diastereomer was the major product, as determined by NMR and X-ray crystallography. The methodology of this reaction is currently being applied to the synthesis of a portion of the tylosin hemiacetal.



12. SYNTHESIS OF PHENYL LACTOLS VIA AN INTERMOLECULAR HECK REACTION, AND ITS POTENTIAL APPLICATION TO THE SYNTHESIS OF (R)-(-)-BACLOFEN

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A Heck reaction of aryl halides or aryl triflates with 2-butene-1,4-diol in the presence of a base and a palladium catalyst coordinated with various ligands produced 4-phenyl-2-hydroxytetrahydrofuran, or phenyl lactols. Variables such as the catalyst, base, solvent, etc. in this reaction were changed to find optimal reaction conditions. The products were then oxidized to phenyl lactones. The reaction conditions needed to produce 4-chlorophenyl lactols were also examined, as the product could be used as an intermediate in a synthetic route to the anti-spastic drug, Baclofen. Reaction conditions in the synthesis of 4-chlorophenyl lactol were improved. The oxidizing agent silver(I) carbonate/celite was found to be more efficient than PCC in oxidizing lactols to lactones. Both lactol and lactone were analyzed by NMR and GC/MS.

13. ENZYMATIC AND CHEMICAL HYDROLYSES OF AN ESTER-CARBONATE DRUG

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Chemists at Lehigh University have developed a new kind of bi-functional pharmaceutical for treating topical pain of cholinergic origin and inflammation, such as might be associated with burns, cuts, abrasions, or even arthritis. These drugs carry a non-steroidal anti-inflammatory (NSAID) segment and a molecular recognition segment for the enzyme acetylcholinesterase (AChE).

With two possible spots in the molecule for hydrolysis, multiple questions arise. Which bond breaks first? Are there pH conditions under which neither bond breaks? In the presence of a cholinesterase, which bond (if any) hydrolyzes first? Preliminary results on this project will be reported.

14. COMPUTATIONAL STUDY OF THE ENE MECHANISM IN NICOTINAMIDE HYDRIDE-EQUIVALENT TRANSFERS

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Transition state structures have been identified for the ene reaction between N-methyl dihydronicotinamide and formaldehyde at RHF/3-21G using Gaussian 03. Transition states were also found at RHF/3-21G for ene reactions of N-methyl 3-R dihydropyridine and formaldehyde, with R = -OH, -NH₂, -COH, -CH₃, and -NO₂. No relationship was found between the electron withdrawing power of R and the thermodynamic or kinetic favorability of the reaction. Several transition states were reoptimized at B3LYP/6-31+G** and were found to vary considerably from the transition structures at RHF/3-21G, to the point that they likely do not represent the same transition state.

15. TOXICITY OF FUNCTIONALIZED CARBON NANOTUBES ON CYANOBACTERIA

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The use of nanomaterials (i.e. carbon nanotubes) in various clinical and biological applications (e.g. as a drug delivery agent for tumor cells) raises questions concerning the human health issues and environmental impact that these nanomaterials may cause. In this study, we are investigating the effect of functionalized single-walled carbon nanotubes (SWNTs) on cyanobacteria (a model system). Functionalized SWNTs were characterized using FT-IR spectroscopy. The nanotubes were added to cyanobacteria cultures to assess whether the presence of SWNTs will affect the biological function of the cyanobacteria. UV-Vis spectroscopy and optical microscopy were used to examine the growth of the cyanobacteria with and without the addition of the functionalized SWNTs. The concentration effect of SWNTs on the growth of cyanobacteria is also examined.

16. ENGINEERING A NEW SELF-ASSOCIATION ABILITY INTO AN APOPTOSIS-REGULATING PROTEIN

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Apoptosis (programmed cell death) is a highly controlled process that requires destructive enzymes called caspases. Inhibitors of apoptosis (IAPs) are proteins that keep caspases inhibited until apoptosis is appropriate. Since caspases are multimeric and contain two catalytic sites, we hypothesize that aggregated IAPs will be more effective inhibitors than monomeric IAPs. We are testing this by creating an IAP that can self-associate on demand. An IAP is being fused to a DNA-binding protein, Hap1, which dimerizes in the presence of DNA. The gene for this IAP-Hap1 fusion protein is being created using recombinant DNA methods. DNA fragments encoding regions of the IAP and Hap1 proteins were amplified by PCR and are being ligated into a pMAL plasmid. This will facilitate recombinant expression of an IAP-Hap1 fusion protein. The new conjugate protein will then be tested for an enhanced ability to inhibit caspases when induced to self-associate by DNA.

17. INVESTIGATION OF OLIGOMERIC STRUCTURE FORMATION IN PHYCOCYANIN: THE TRIMER ↔ MONOMER TRANSITION

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Phycocyanin is a light harvesting protein from cyanobacteria consisting of alpha-beta heterodimer in which the alpha subunit contains one chromophore and the beta subunit contains two chromophores. The alpha-beta heterodimer may oligomerize into several structures: a hexamer, trimer, or monomer of heterodimers. In this study the transition between monomeric and trimeric structure will be examined using stopped flow absorption spectroscopy. Potential mechanisms of oligomeric structure formation and dissociation will be discussed.

18. DNA INTERACTIONS OF AN ANTITUMOR-ACTIVE RUTHENIUM COMPOUND

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Transition metal complexes such as cisplatin have been in use as chemotherapeutic drugs. The mechanism of their action is believed to involve covalent cross-linking of DNA strands, causing inhibition of the normal processing of this key biological molecule and induction of apoptosis. However, the harmful side effects of and drug resistance to cisplatin have caused researchers to focus their attention on other metal complexes. Our work explores the potential for covalent DNA-binding as a plausible mechanism for the antitumor activity of a metal complex, N,N',N'' -trimethyl-1,4,7-triazacyclononane-ruthenium-trichloride (noted hereafter as tacn-RuCl₃), tacn-RuCl₃. Evidence from proton NMR spectroscopy suggests that tacn-RuCl₃ is capable of binding to all four nucleosides. Time-dependent binding studies with double-stranded salmon testes DNA were monitored by UV-Vis and graphite furnace atomic absorption spectroscopy (GFAAS). Taken together, these data provide evidence to support that covalent interactions between tacn-RuCl₃ and DNA may be relevant to antitumor activity.

19. RUTHENIUM HYDRIDE HYDROGENATION CATALYSTS WITH BISPHOSPHINOMETALLOCENE LIGANDS

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Syntheses of Cp(P-P)RuCl species (P-P = bis(diphenylphosphino)ferrocene (dppf), bis(diisopropylphosphino)ferrocene (dippf), bis(dicyclohexylphosphino)ferrocene (dcpf), bis(diphenylphosphino)ruthenicene (dppr), bis(diphenylphosphineo)osmicene (dppo)) are described. In addition, a new process was developed for the conversion of the chloride to the corresponding hydride using NaBH₄ at room temperature. The new chlorides and hydrides were characterized by ¹H and ³¹P NMR and electrochemistry was performed on each compound. The ionic homogeneous hydrogenation of three different ethylenepyrrrolidinium tetrafluoroborate compounds was performed using these compounds. The effect of altering the P-P ligand on the hydride transfer ability of the complex was examined using time restrained, stoichiometric reactions.

20. TUNGSTEN COMPLEXES OF A CHIRAL C₂-SYMMETRIC TETRAAMINE LIGAND

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Because aromatic molecules are abundant, are relatively inexpensive, and come in a wide variety of substitutions, these molecules have great potential as starting materials in many industrial and pharmaceutical processes, but they do not tend to readily undergo addition reactions. By making certain varieties of electron-rich metal fragments, the goal of this project is to synthesize enantioselective dearomatization agents that will promote aromatic addition reactions. A C₂-symmetric chiral pyridine-based diimine, *trans*- N,N' -bis(pyridin-2-ylmethylene)cyclohexane-1,2-diimine, was synthesized in 75.0% yield. The pyridine-based diimine was reduced to give picchxn (picchxn = *trans*- N,N' -bis(pyridine-2-ylmethyl)cyclohexane-1,2-diamine) in 80.8% yield. The picchxn ligand was complexed with tungsten hexacarbonyl to produce (κ^3 -picchxn)W(CO)₃ with 87.8% yield. [(κ^3 -picchxn)W(CO)₂(NO)]PF₆ was synthesized from (κ^3 -picchxn)W(CO)₃ in 93.2% yield. [(*cis*- α -picchxn)W(CO)(NO)]PF₆ was synthesized from [(*cis*- α -picchxn)W(CO)₂(NO)]PF₆ in 95.9% yield. Compounds were characterized by ¹H NMR spectroscopy, infrared spectroscopy, and CHN analysis. Future research will be devoted to exploring the reactivity of the metal fragments.

21. INVESTIGATION OF THE SPECTROSCOPY AND REDUCTION POTENTIAL CHEMISTRY OF CRYPTOCHROME 1 FROM *VIBRIO CHOLERAE*

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Cryptochrome is a member of the blue-light photoreceptor family, a family that also includes DNA Photolyase. VcCry1, a cryptochrome in the DASH subfamily from *Vibrio cholerae*, has been shown to repair photoinduced cyclobutane dimers in single stranded DNA. We have developed a procedure to generate the one electron oxidized species, the semiquinone state, of the flavin cofactor. Preliminary results indicate that the semiquinone state is stabilized by the presence of substrate, and its absorption spectrum undergoes an electrochromic shift upon substrate binding. Both of these findings indicate considerable similarities between VcCry1 and *E. coli* DNA Photolyase.

22. SEPARATION AND DNA BINDING REACTIONS OF DIRHODIUM COMPOUNDS

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Dirhodium (II,II) carboxylate and acetamidate complexes have been shown to have significant anti-tumor activity^{1,2} with DNA as a potential biological target³. Modifications to the carboxylate and acetamidate ligands have been shown to affect the rate of DNA-binding of these complexes³. A sample of one of these anti-tumor active compounds, dirhodium(II,II)tetratetrafluoroacetamide (**Rh4**), has been synthesized by our collaborators and been studied previously in this lab. Although this compound does bind covalently to DNA, at maximum binding only 25-30% of the rhodium is bound to DNA⁴. One possible explanation of this limited DNA-binding is that Rh4, as supplied, may be a mixture of components. The goal of this project was to determine if the Rh4 sample (as supplied) is a mixture of components and, if so, to separate the components, determine their stability in solution, and measure their individual ability to covalently bind duplex DNA over time.

23. STOPPED FLOW STUDIES OF HEXAMER FORMATION AND DISSOCIATION IN PHYCOCYANIN

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Phycocyanin, isolated from cyanobacteria, is an oligomeric protein that functions in the phycobilisome, or light-harvesting antennae. The oligomeric structure of phycocyanin is based on an alpha-beta heterodimer in which the beta subunit contains two and the alpha subunit contains one phycocyanobilin, a tetrapyrrole chromophore. There are three stable oligomeric forms of the protein: a hexamer of heterodimers, trimer of heterodimers, and a monomer of heterodimers. Each of these states have unique spectroscopic signatures. In the cell, phycocyanin is spectroscopically indistinguishable from a hexamer state. The oligomeric structure of the protein can be controlled with urea. We report the kinetics of the transition between the hexamer and trimer states, and we will discuss potential mechanisms for the formation and dissociation of oligomeric structures.

24. DETERMINATION OF DNA STRUCTURE: EFFECTS OF ⁶S

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This study is focused on determining the structural changes that occur in DNA following the incorporation of 6-thioguanine (⁶S). This chemotherapy agent has been used in the treatment of childhood acute lymphoblastic leukemia, and in a number of other medical applications due to its toxicity to rapidly dividing cells.

Using previously collected ¹H-NMR data, we analyzed the NOESY and COSY spectra of the control 11-mer duplex. Sequence specific assignments were made in SPARKY, and XPLOL was then used to generate a three-dimensional model of the DNA with NMR distance restraints. Once accurately modeled this control duplex can be used to discern the conformational changes induced by ⁶S.