Chemistry

PHOTOSWITCHABLE ARYLAZOPYRAZOLE LIGANDS: SYNTHESIS AND COORDINATION CHEM. Keset Y. Ghebreyessus and Janay I. Little, Department of Chemistry and Biochemistry Hampton University, Hampton, VA 23668. Novel palladium(II) and platinum(II) coordination complexes incorporating pyridine and benzothiazole functionalized photo-switchable arylazopyrazole ligands were synthesized and characterized. The photo-physical properties of the ligands and their corresponding metal complexes have been investigated. The effect of the nature of the ligands and type of metals on the rate of the *cis*-to-*trans* photo-isomerization process has also been explored. The ligands and the metal complexes exhibit strong absorption bands in the UV region, and weak bands in the visible region. Upon irradiation with UV-light (λ = 365 nm) these compounds clearly undergo efficient and almost quantitative *trans*-to-*cis* photo-isomerization of the azopyrazole unit followed by the reverse *cis*-to-*trans* isomerization upon standing under normal light. The results indicate that the percent conversion of the *trans*-to-*cis* isomerization is highly dependent on the substitution pattern on the pyrazole ring, which also has a significant influence on the electronic properties of the compounds. (Supported by: the Hampton University Faculty Research Fund, NSF CREST Center and PREM)

PROGRESS TOWARD A "GREEN" REDUCING AGENT. Charles M. Bump, Department of Chemistry and Biochemistry, Hampton University 23668. Solutions of freshly brewed green tea have been successfully used in the synthesis of gold and silver nanoparticles. During that process, the tea reduces metal ions (Au^{3+}, Ag^{+}) to their elemental state and caps those atoms with a large organic molecule that prevents the aggregation and precipitation of colloidal metal. Among the more conventional reducing agents used in the synthesis of nanoparticles is $NaBH_4$. That same reducing agent is widely used for the conversion of aldehydes and ketones to alcohols. We are beginning an investigation on expanding the use of green tea for the reduction of aldehydes and ketones. Some of the difficulties to be addressed include the poor solubility of ketones in aqueous media (e.g. tea), determining the length of time required for the reduction to take place, and the isolation of the reduction product.

MICROWAVE-ASSISTED SYNTHESIS AND CHARACTERIZATION OF METALLIC NANOMATERIALS Peter N. Njoki, Department of Chemistry & Biochemistry, Hampton University, Hampton VA 23668. Laboratory microwaves are becoming common tools in research and teaching laboratory. Compared to

conventional means of heating, microwaves provide shorter reaction times, better reproducibility, and enhanced reaction control. The key component of microwave-assisted heating is that nanoparticles synthesis can be completed within minutes thereby saving time and energy. Nanomaterials possess novel properties as the size of particles decreases to nanoscale. To understand and exploit these novel properties, we need to develop effective strategies to synthesize nanoparticles with controllable size, shape, and composition. In this presentation, we focus on synthesis of gold and silver nanoparticles due to their unique optical properties and ease of fabrication. This presentation describes results of a microwave-assisted irradiation method aimed at developing the ability to control the size and composition of gold and silver nanoparticles. We will also discuss applications of these nanoparticles in fuel cell and forensic analysis. An array of analytical techniques such as transmission electron microscopy and UV-Vis spectrophotometry were used for the characterizations.

ENGAGING INQUIRY-BASED STUDENT LEARNING USING COMPUTATIONAL CHEMISTRY IPAD APPS IN ORGANIC CHEMISTRY LABORATORIES. Michelle K. Waddell, Charles Bump, Godson Nwokogu & Edmund Ndip, Dept. of Chem. and Biochem., Hampton Univ., Hampton VA. 23668. Inquiry-based classrooms encourage students to explore and understand their world using scientific methods. Spartan has been used to integrate computational chemistry into undergraduate chemistry curriculum. Computers and modeling software were purchased for use in chemistry courses. However, calculations using Gaussian and Argus Lab software to minimize energies of organic molecules routinely ran for several hours and are not feasible for use in the organic laboratory sections. The free website 4 Mol D was adopted for its quick efficient calculations. This project compares organic chemistry students' comprehension of inquiry-based learning of computational chemistry 3D models of various experiments using 4 Mol D and the iPad mini iSpartan app. Student outcomes were assessed in retrospective web-based surveys administered on-line through Blackboard TM 9.0 to access comprehension of the material, level of success in achieving learning outcomes and technical ability to utilize the molecular modeling applications. Results indicated that students were more comfortable using the iPad minis due to its ease of use and reliability of access. Student data collected from iPad minis and 4 Mol D was comparable to one another.

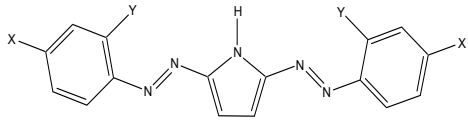
GC/MS QUANTIFICATION OF THE BIOFUEL POTENTIAL OF ALGAE**.** Grant A. McClure & Todd Allen, Dept. of Biol. and Chem., Liberty Univ., Lynchburg VA. 24502. Microalgae has the potential to be used as an alternative to petroleum-based feedstock necessary for

transportation fuels. Several companies are researching cost-effective ways to optimize algae growth and harvesting techniques in an effort to convert the lipid fraction of the algae biomass into various types of fuels. The ability to accurately quantify the lipid content of algae is essential to evaluating the fuel potential. A validated GC/MSD (Gas Chromatography coupled with Mass Spectrometric Detection) method was previously developed for the quantitative analysis of the biofuel potential in algal samples provided in lyophilized and filtered mediums. Companies are exploring new oil extraction techniques to maximize the harvest efficiency of the oil from the algae. The new oil extract required additional steps be taken in the beginning stages of the sample preparation to accommodate the unique matrix. After the additional steps for the new matrix, all subsequent steps merge with the other matrices preparation method. Results will be presented.

MICROWAVE-ASSISTED SYNTHESIS AND CHARACTERIZATION OF METALLIC NANOMATERIALS Peter N. Njoki, Department of Chemistry & Biochemistry, Hampton University, Hampton VA 23668. Laboratory microwaves are becoming common tools in research and teaching laboratory. Compared to conventional means of heating, microwaves provide shorter reaction times, better reproducibility, and enhanced reaction control. The key component of microwave-assisted heating is that nanoparticles synthesis can be completed within minutes thereby saving time and energy. Nanomaterials possess novel properties as the size of particles decreases to nanoscale. To understand and exploit these novel properties, we need to develop effective strategies to synthesize nanoparticles with controllable size, shape, and composition. In this presentation, we focus on synthesis of gold and silver nanoparticles due to their unique optical properties and ease of fabrication. This presentation describes results of a microwave-assisted irradiation method aimed at developing the ability to control the size and composition of gold and silver nanoparticles. We will also discuss applications of these nanoparticles in fuel cell and forensic analysis. An array of analytical techniques such as transmission electron microscopy and UV-Vis spectrophotometry were used for the characterizations.

EFFECTS OF SUBSTITUENTS AND BRIDGE LENGTH ON NLO PROPERTIES OF A SERIES OF BIS AZO DYES. Edmund Moses N. Ndip, David S. Barnes & Binal Patel. Department of Chemistry and Biochemistry, Hampton University, Hampton, VA 23668. In the present study, the effect of variations in donor – acceptor pairs on frequency dependent nonlinear optical properties has been investigated. Semi-empirical calculations of the frequency-dependent linear polarizability, α, the second, β- and third, γ-order hyperpolarizabilities at the fundamental (1028 nm) and other wavelengths were achieved by applying the *ab initio* time-dependent coupled perturbed Hartree -Fock

(TDHF) method at the Restricted Hartree- Fock (RHF) level using routines contained in MOPAC2012 program for various model systems shown below (1-10). The D-π-D structures were found to have lower bandgaps (6.585 – 7.004 eV) as well as significantly lower second-order hyperpolarizability values compared to values for A-π-A, A-π-D, or D-π-A structures. This work was funded in part by Hampton University's NSF CREST (ACLaSS) and HRD 1238838.



Compound #	X	X	Y	Y	Type
1	H	H	H	H	
2	CO_2H	CO_2H	H	H	A-π-A
3	NH_2	NH_2	H	H	D-π-D
4	CO_2H	NH_2	H	H	A-π-D
5	OH	OH	H	H	D-π-D
6	CO_2H	OH	H	H	A-π-D
7	NH_2	OH	H	H	D-π-D
8	H	H	OH	OH	No type
9	NPH_2	NPH_2	H	H	D-π-D
10	N-Carbazoyl	N-Carbazoyl	H	H	

CHEMISTY AND SPECTROSCOPY IN KBR MATRICES, T.C. DeVore, Dept of Chem. and Biochem., James Madison University, Harrisonburg VA 22807. Fifty years ago, several methods for trapping ions in KBr crystals were discovered. The IR spectrum of these ions could then be investigated and chemical reactions involving these ions could be investigated by heating the crystal. One way to use this method in the chemistry labs is to investigate the spectra of isoelectronic series of molecules. One example of this presented is the changes in the bond strengths for 16 electron linear molecules BO_2^- ,

CO_2, and NCO^-. The IR spectrum of BO_2^- shows a clear isotope effect and can also be used to measure the isotopic abundance of boron. A similar exercise can be done with the isoelectronic tetrahedral molecules/ ions BH_4^-, CH_4, and NH_4^+. The thermal decomposition of the oxalate ion in KBr produced by allowing an aqueous solution containing 1% sodium oxalate- 99% KBr to evaporate to dryness. Heating the solid to 775 K produced 4 new IR bands that may arise from $COCO_3^{2-}$ which has been predicted to be an intermediate in this decomposition.

CHARACTERIZATION OF ALGAL PIGMENTS USING ABSORBANCE AND FLUORESCENCE**.** C. M. Fleming, Z. J. Schreiber & T. M. Allen, Department of Biology and Chemistry, Liberty University, Lynchburg VA 24502. The effectiveness of identifying different types of chlorophyll within microalgae is vital in predicting not only the lipid content, but also understanding why chlorophyll is contaminating the hexane layer during the sample preparation process. This contamination of chlorophyll and other proteins inhibits the extracted lipids from immediately being used for biofuels. A comparison of absorbance and fluorescence in both the organic and aqueous layers were measured to analyze the ratio between extracted and non-extracted pigments found in the organic layer.