

Chemistry

SYNTHESIS OF METAL ORGANIC FRAMEWORKS AND THEIR ACTIVATION KINETICS. Barbara A. Reisner & W. Tyler Price, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. Metal organic frameworks derived from the hydrotris(1,2,4-triazolyl)borate ligand were synthesized from water, dimethylformamide (DMF) and isopropanol (IPA). $\text{Na}[\text{BH}(\text{C}_2\text{H}_3\text{N}_3)_3]\cdot\text{solvent}$ (solvent = H_2O , DMF, IPA) crystallize as a porous framework with the distorted primitive cubic (pcu) topology. Solvent molecules occupy the framework pores. The solvent of crystallization can be removed by heating. Isothermal thermogravimetric analysis shows that solvent loss is consistent with a 1-D diffusion mechanism. Variable temperature powder X-ray diffraction (PXRD) data show some loss of crystallinity upon desolvation, indicating some framework decomposition. These materials adsorb water from the atmosphere. The structures of $\text{Na}[\text{BH}(\text{C}_2\text{H}_3\text{N}_3)_3]\cdot\text{solvent}$, their thermal behavior, stability and the kinetics of solvent loss of will be reported.

EVALUATION OF NAPHTHALIMIDE-TAGGED RUTHENIUM (II)-ARENE COMPLEXES AS POTENTIAL ANTICANCER AGENTS. Kesete Y. Ghebreyessus¹, Ashley N. Peralta¹, Meena Katdare², Krishnan Prabhakaran², & Shanthi Paranawithana¹, ¹Department of Chemistry, & ²Skin of Color Research Institute, Hampton University, Hampton, VA 23668. New ruthenium (II)-arene complexes bearing ligands that incorporate a biologically active 1,8-naphthalimide moiety have been synthesized and characterized by NMR, IR, and electrospray (ESI-MS) mass-spectrometer. The anticancer activities of the ligands and their corresponding ruthenium (II)-arene complexes were further evaluated *in vitro* against CRL7687 (human melanoma skin cancer) and CA-M75 (normal skin melanocyte) cell lines. All of the compounds exhibit significantly high anticancer activity, with IC_{50} values of $<1\text{mM}$. The high anti-proliferative activity of the new ruthenium (II)-arene complexes against the human melanoma skin cancer cell line has indicated their potential for further development as anticancer drugs. Furthermore, as DNA is considered to be one of the main biological targets for ruthenium(II)-arene complexes, their interaction with DNA were followed by UV-Vis and fluorescence spectroscopy, and gel electrophoresis assay. The results of the absorption and fluorescence titrations, and gel electrophoresis assay suggest that these new complexes bind to DNA moderately, presumably interacting through an intercalative mode. (Supported by the Hampton University Faculty Research Fund and NSF CREST center).

WinPSSP: A REVAMP OF THE CRYSTAL STRUCTURE DETERMINATION PROGRAM PSSP WITH EDUCATIONAL PERSPECTIVES. S. Pagola¹, A. Polymeros² & N. Kourkoumelis³, ¹Applied Science Dept., College of William & Mary & Applied Research Center, 12050 Jefferson Avenue, Newport News, VA, 23606, ²Department of Physics, University of Ioannina, 45110, Ioannina, Greece, ³Department of Medical Physics, Medical School, University of Ioannina, 45110, Ioannina, Greece.

PSSP is a direct-space methods program for the crystal structure solution of molecular solids from X-ray powder diffraction. *PSSP* uses the integrated intensities of the powder diffraction peaks extracted in a Le Bail fit of the data, the geometry of the molecules from databases or molecular geometry optimizations and the simulated annealing algorithm to locate the molecules (asymmetric unit) in the lattice. *WinPSSP* is based on the *PSSP* source code. A new GUI (graphical user interface) suitable to familiarize undergraduate college students to crystal structure solution from powders has been added, and work on advanced features for non-routine problems, such as crystal structure solution of co-crystals and other materials with more than one crystallographically independent fragment in the asymmetric unit is in progress. Our goals are: (1) to optimize the code for faster runs in windows-based operating systems, and (2) to facilitate additional educational features to introduce the crystallographic and diffraction nomenclature in undergraduate courses.

COMPARISON OF NEGATIVE ION ELECTROSPRAY IONIZATION EFFICIENCIES FOR A DIVERSITY OF SMALL ACIDIC MOLECULES WITH WIDELY VARYING pK_a 'S. James M. Mattila, Shelsea A. Hurdle & Christine A. Hughey, Dept. of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. Negative ion electrospray (ESI), an ionization technique that selectively ionizes acidic molecules by deprotonation, has not been studied as extensively as positive ion ESI. As a result, our long-term goals are to elucidate the mechanisms of ionization and to develop a model that predicts ESI response for a diversity of small acidic molecules with a wide range of acidities. To date, negative ion ESI studies have largely focused on two compound classes: phenols and benzoic acids. Here we measure the ionization efficiencies of ~100 compounds by triple quadrupole mass spectrometry. The compounds were systematically selected among *n*-carboxylic acids, benzoic acids, phenols, thiophenols, acetanilides, indoles and steroids. The pK_a 's for compounds studied ranged from -0.78 to 20. Within each class, compounds substituted with electron-withdrawing groups (EWGs), such as CF_3 , NO_2 and CN , generally exhibited higher responses than compounds with electron donating groups (EDGs), such as $-OCH_3$ and NH_2 . Compounds with SH and $NH(CO)CH_3$ exhibited higher than expected responses. This larger data set further supports our initial hypothesis that functional groups that withdraw electrons from the benzene ring through induction and/or resonance stabilization makes it easier to remove the proton during ionization. NSF CHE-1307226 supports this work.

FORMATION OF NANOPARTICLES USING GREEN TEA EXTRACT. Michelle K. Waddell¹, Jermarion Griffin² & Amira Manes³, Department of Chemistry, ¹Hampton University, ²Kecoughtan H.S. Hampton VA, & ³King's Fork H.S. Suffolk VA. Pollution of the world oceans by oil has become a major environmental problem. As a result, numerous methods are employed to remove these contaminants. Surfactants are used in various stages of oil spill clean-up by the petroleum industry. The critical micelle concentration (cmc) of surfactants in solution must be reached to achieve maximum absorption. However, there is a concern about the wide spread use of

surfactants due to their ability increase the diffusion of other environmental contaminants. Nanoparticles that incorporate a minimum concentration of surfactants which can effectively disperse oil in aqueous media would be an innovative advancement for the petroleum industry. This research project will occur in two phases. The first phase involves synthesis of iron magnetic nanoparticles coated with capping agents and ionic surfactants. Organic capping agents (green tea extract) and surfactants will serve a dual purpose. First, it will protect the easily oxidized iron center and assist in micelle formation of the nanoparticles. Secondly, the ionic surfactants will form emulsions with organic contaminants in aqueous media. Due to the magnetic characteristic of these nanoparticles, they will be used to remove organic contaminants noninvasively. A series of studies were to be conducted on the effectiveness of forming iron nanoparticles in various solvents and different pH levels (5, 6, 7 and 8) using tetrabutylammonium iodide or lecithin as a surfactant. The results of this research will be presented in this paper. (Supported by: NSF HBCU-UP ACE Nano HU HRD-1238838).

OPTIMIZING THE RATIO OF GREEN TEA TO SILVER NITRATE IN THE FORMATION OF SILVER NANOPARTICLES. Charles M. Bump, Brandon Peck & Kayla Davis, Department of Chemistry, Hampton University 23668. Nanoparticle synthesis requires the reduction of a metal salt to the elemental form of the metal in the presence of a “capping agent” that prevents aggregation of the metal in an amorphous mass. Green tea has been advanced as an environmentally friendly and fast-acting reducing agent while simultaneously serving as the capping agent. We report the amount of silver ion that can be converted to silver nanoparticles from a fixed amount of green tea.

ASSESSING THE ACTIVITY OF ANTIBACTERIAL POLYMERS. O. Oyesanya, Department of Chemistry, Norfolk State University, Norfolk VA 23504. Quaternized poly(4-vinylpyridine) (P4VP) and poly(4-vinylpyridine-co-styrene) (P4VP-S) are polymers with antibacterial properties against both Gram-positive and Gram-negative bacteria. The syntheses of the two polymers were carried out using controlled free-radical polymerization in the presence of benzoyl peroxide (BPO) and 2,2,6,6-tetramethylpiperidine-*N*-oxyl (TEMPO) followed by quaternization with 1-bromobutane. Polymers were characterized by nuclear magnetic resonance (NMR) spectroscopy, Fourier transform infrared (FTIR) spectrophotometry, and ultraviolet-visible (UV-Vis) spectroscopy. Differences in the antibacterial activity of the two polymers were investigated due to differences in the number of pyridinium groups on polymers. Antibacterial assessments were conducted by interaction of P(4VP-BB) and P(4VP-S-BB) with Gram-positive bacteria (*Staphylococcus aureus* and *Enterococcus faecalis*) and Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*) in aqueous solutions. Results reveal that the polymers are significantly effective against the test bacteria.

SOLVENT EFFECTS ON THE LINEAR PROPERTIES OF A SERIES OF CENTROSYMMETRIC D- Π -D ARYL STYRYL ORGANIC SEMICONDUCTORS. E. M. N. Ndip¹ & C. E. Dula,² ¹Department of Chemistry & Biochemistry, Hampton University, Hampton, VA 23668 ²Washington University School of Medicine, The Edward Mallinckrodt Department of Pediatrics, St. Louis, MO 63110. This work is part of our ongoing investigation on the design, synthesis, and laser spectroscopic characterization of variously bridged aryl styryl heterocyclic systems for molecular electronics. We have investigated solvent effects on the linear absorption spectra, λ_{max} (bandgap, ΔE), transition dipoles, and oscillator strengths of a series of furan, thiophene, and pyrrole vinylene bridged donor- π -donor aryl styryl systems at the semi empirical level using ZINDO-CI methodology. The solvents used in these studies included: acetonitrile, chloroform, methanol and toluene. The difference in absorptions wavelengths between gas phase and solvated model systems vary from ± 20 nm for the thiophene systems to ± 15 nm for the furans and ± 10 nm for the pyrrole systems. Solvent effects are less noticeable in the azo-bridged systems than in the vinylene-bridged systems. Support for this work was provided through Hampton University's NSF CREST CLaSS (Materials and Modeling IRG) grant (HRD-0734635).

CAN DSC BE USED TO DETERMINE THE ENTHALPIES OF FORMATION FOR THE 3d TRANSITION METAL OXALATES? R. Snell-Feikma & T.C. DeVore, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. On paper, the thermal decomposition of first row transition metal oxalates occurs in one step to produce well established products so it should be possible to use these reactions to determine the enthalpies of formation for these compounds. In practice, secondary reactions between the gaseous and solid products or between the gaseous products often occur producing a mixture of products. Attempts to fully oxidize the products by doing the decomposition in static air also failed to give consistent values. However, adding a flameless combustion catalyst (CuO) and using slow scans (2 K min⁻¹) in static air produced values for the enthalpies of formation that agreed to within 1% of the more reliable values reported previously.

Posters

FABRICATION OF MAGNETIC IRON NANOPARTICLES FOR OIL SPILL REMEDIATION BY FACILE MICROWAVE PROCESS. Breyinn N. Loftin, & Michelle K. Waddell PhD, Dept. of Chemistry, Hampton University, Hampton VA 23668. Recently, innovative nanotechnology approaches have gained attention for oil spill remediation. Magnetic nanocomposites have added magnetic properties that allow for the recovery of the deployed nanomaterial. Using nanomaterials for oil spill remediation offers a more cost and time efficient method. Nanomaterials are also more feasible than using sorbent materials and bioremediation. The superparamagnetic properties of iron nanoparticles make these materials ideal for use in oil spill remediation. In this presentation, the fabrication of magnetic iron nanoparticles by

facile microwave process is demonstrated. The microwave approach is more effective for large-scale production of high quality nanoparticles. The procedure consisted of making a precursor solution to be used in the microwave reactions. The precursor was obtained by using $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ and HCl with a series of capping agents lecithin, green tea extract, pure tannic acid, and poly(bisphenol A carbonate). The capping agent combines with lecithin to form micelles around the iron core to form the nanoparticles. A progression of microwave trials were ran in order to observe any effects on the formation of nanoparticles. The resulting products were characterized using UV-Vis spectroscopy. Iron nanoparticles usually absorb light in the 400-600nm region. Results indicated that nanoparticles are present in the reaction mixture of the tannic acid.

UNIQUE CHARACTERISTICS OF POLYOXOMETALATES AND THEIR SYNTHESIS. M. Smith, S. Puckett, O. Wampler, J. D. Powell, School of Natural Sciences & Mathematics, Ferrum College, Ferrum VA 24088. Polyoxometalates are clusters of highly oxidized early transition metals covalently bonded to oxygen atoms and sometimes other heteroatoms. These molecules usually contain a caged structure that encloses a smaller molecular ionic unit. They most commonly contain molybdenum and tungsten, which when combined with other metals give a wide variety of physical and chemical properties. Their complex caged structures can be rearranged by adjusting concentration, pH, and counter ions. Because of their high molar mass, polyoxometalate compounds are best characterized in the crystalline state by FT-IR and single-crystal x-ray diffraction. UV-visible spectrophotometry and electrochemistry provide supplementary characterization in solution. Lacunary polyoxometalate structures can be formed by the removal of at least one metal vertex from the cage. The remaining ions retain a high negative charge which makes them highly reactive towards metal ions and other Lewis bases. Sample reactions were observed through a series of tests on solutions containing different polyoxometalate ions. Synthesis and characterization of new polyoxometalates may produce compounds with unique chemical and physical properties for future applications.

Computer Science

A STUDY ON THE CHALLENGES OF BUILDING A TRUSTWORTHY NETWORK. Yen-Hung Hu, Department of Computer Science, Norfolk State University, Norfolk VA 23504. Building a trustworthy network faces several severe challenges adhering to the current computing infrastructure (e.g., computer architectures, network architectures, operating systems, communication protocols and applications, and so on.). Since hardware and software of a network system are from various vendors and manufacturers, it is very difficult to assess trustworthiness of any system without proper criteria and methods. Meanwhile, misconfigurations of hardware and software by end-users will worsen this issue even though such hardware and software are well prepared by following appropriate industrial security guidelines. Therefore, concerns regarding criteria and methods for assessing trustworthiness should