CHEMISTRY PAPER ABSTRACTS

SYNTHESIS, CHARACTERIZATION AND REACTIVITY STUDIES OF COPPER (II) AND NICKEL (II) COMPLEXES. *NIHARIKA BOTCHA*, UNIVERSITY OF ALABAMA IN HUNTSVILLE. NIRUPAMA SINGH, AMBIOPHARM INC. ANUSREE MUKHERJEE, THE UNIVERSITY OF ALABAMA IN HUNTSVILLE.

The constantly increasing demand for energy and fuel resources requires the development of new energy solutions that are more sustainable and address the need for energy efficiency and conservation. Coordination complexes of late transition metals bound by nitrogen rich ligands are very important because of their pivotal roles in catalytic applications. Tetradenatate ligands from the bispicen family with amine and pyridine functionalities (N2/Py2) have also received significant attention for their role in hydrocarbon oxidation with high selectivity. These ligands are also attractive candidates for designing homogeneous catalysts as ease of synthesis allows systematic investigation of structural-functional relationship of the catalysts. They efficiently catalyze most of the organic transformations occurs in living systems under mild conditions with nontoxic oxidants such as O2 or H2O2 to oxidize a wide range of molecules, usually in a very selective manner. Thus, we can take inspiration from these natural phenomenon’s and attempt to develop new catalysts that will ideally oxidize a wide array of organic molecules using cheap and environmentally benign oxidants. In our group synthetic mononuclear copper (II) and nickel (II) metal containing model complexes were synthesized and characterized using different spectroscopic techniques.

IDENTIFICATION OF ODOROUS VOLATILE COMPOUNDS IN RECYCLED PLASTIC RESINS. *JON FULLER*, ZANE VICKERY AND SHAOYANG LIU, TROY UNIVERSITY. JASON COLLEY, UNIVERSITY OF GEORGIA. DAVID NORMAN, EMORY UNIVERSITY.

The process of recycling plastics into usable material is an important part of waste management and in particular the reduction of solid waste. Although recycled plastics provide a low-cost and environmentally friendly alternative material for many everyday objects, there are several factors that limit the desirability of recycled plastics. Most notably among these is the presence of undesirable odors which are caused by volatile organic compounds (VOCs) in much of the recycled material. In this work, headspace solid-phase microextraction (HS-SPME) coupled with the gas chromatography-mass spectrometry (GC-MS) method was used to analyze volatile compounds from recycled plastic resins with odors. The established analysis methods have proven to be sensitive and relatively comprehensive to volatile compounds from plastic resins. Retention index (RI) and mass spectra of suspected odor-causing compounds were acquired and compared to those from standards to identify the culprit compounds behind the odor of the plastic resin. Notable amounts of D-limonene, octanal and nonanal were found in the odorous resins. However, some other odorous compounds presenting in other recycled plastic samples, including 2-acetyl-1-pyrroline, 2-methylisoborneol, 2,4,6-Trichloroanisol, γ-nonalactone, γ-necalactone, patchouli alcohol, γ-dodecalactone and vanillin were not detected in this work. This research is performed in an attempt to discover the relationship between the unpleasant odors of recycled resins and the specific volatile compounds they contain. By correctly identifying the specific VOCs that cause the unpleasant odors, further research may be undertaken to remove them or otherwise mitigate their odorous presence and thereby aid the plastic recycling industry in improving product quality.

THE PYROLYSIS OF BP TARBALLS. *AMBER SMITH*, JACKSONVILLE STATE UNIVERSITY.

We have used thermal pyrolysis to analyze oil residue in tarballs collected at Gulf Shores, Alabama, after the April 2010 BP disaster. The oil residue was extracted from tarballs with dichloromethane. On average, BP tarballs contained between 10-18% of a semi-solid mixture of high-molecular weight hydrocarbons, resins, and asphaltenes. Such mixtures cannot be analyzed using conventional GC methods. Therefore, approximately 100 mg of the residue was encapsulated in an evacuated Pyrex tube and pyrolyzed at 440 °C. In these conditions, oil residue is decomposed into hydrogen and saturated/unsaturated hydrocarbons. Each saturated hydrocarbon is formed together with several unsaturated compounds containing the same number of carbon atoms, such as decane and isomers of decene. During pyrolysis, mostly straight-chain alkanes are generated whereas both straight-chain and branched alkenes are obtained. The infrared spectra of tarball extracts show the presence of small amounts of hydroxyl groups indicating that the oxidative decomposition of the oil residue in marine environment is very slow.

OPTIMIZATION OF A TETRACHLOROETHYLENE-METHYL METHACRYLATE COPOLYMER SYSTEM UNDER PH7 BUFFER. *LOREN CHEATWOOD*, JUSTIN TINKER AND DONNA PERYGIN, JACKSONVILLE STATE UNIVERSITY.

We tested different ratios of tetrachloroethylene (TCE) and methyl methacrylate (MMA) under a pH7 phosphate buffer to determine the optimal matrix composition for polymerization. Percent MMA varied from 0% to 100% by volume, in 10% increments. We achieved polymerization of the copolymer above 60% MMA. The optimal matrix, resulting in an extremely hard polymer, was comprised of 80% MMA, and 20% TCE. When the process was repeated without buffer, polymerization was slower under otherwise identical conditions. Polymerization was verified by IR and DSC. DSC confirmed a higher decomposition temperature for the copolymer, relative to MMA only, demonstrating a more stable system for the copolymer, and indicating a stronger matrix for this system.

THE LIFE AND LEGACY OF RACHEL CARSON. *AMANDA COFFMAN*, UNIVERSITY OF NORTH ALABAMA.

The courageous work of Rachel Carson inspired chemists to become more conscientious, the government to consider instigating regulations and the Environmental Protection Agency, and the formation of disciplines such as environmental biology and chemistry as well as Industrial Hygiene. Rachel Louise Carson used her skills as a scientist to collect data and evidence that illustrated the misuse and overuse of pesticides, particularly, dichlorodiphenyltrichloroethane (DDT). Additionally, she employed her talent as a New York Times bestselling author to publish her findings in the 1962 book Silent Spring. After defending her findings, in May 1963, Rachel Carson appeared before the Department of Commerce and requested the establishment of regulations for the use of harmful pesticides. Ten years later, the Environmental Protection Agency was commissioned, which immediately banned DDT. Presented here is a short synopsis of the life, legacy, and work of Rachel Carson, including the various pesticides analyzed, and the biomagnification of pesticide concentration levels that had been identified in the soil, water, and bird specimens. Her interdisciplinary contributions as a scientist, author, and humanitarian were directly and indirectly instrumental in promoting Green Chemistry Practices and Environmental Chemistry.

CHEMISTRY POSTER ABSTRACTS

GENERATING A STATE DIAGRAM OF LANGMUIR FILMS OF QUANTUM DOTS. *CUONG NGUYEN* AND JEFFREY WEIMER, UNIVERSITY OF ALABAMA IN HUNTSVILLE.

We present a state diagram to create Langmuir films of quantum dots (QDs). The approach is to deposit QDs that are dissolved in an organic solvent onto a water sub-phase as a free-standing Langmuir film, where they subsequently self-assemble. By controlling the concentration of the QDs and the volume of deposition, we create different structures and patterns in the films. Fluorescence from the films is imaged at macroscopic scales using a digital camera, and microscopic images are taken using Brewster angle microscopy (BAM). Terms such as coffee ring, splatter, and uniform spread are applied to define the macroscopic film structure qualitatively. Quantitative calculations are made of the minimum area spread by the solvent and the area ratio of the QDs relative to a theoretical monolayer. Histogram analysis from the camera images determines the relative populations of QDs in a monolayer versus multi-layers. The BAM images define the state of self-assembly at micron scales. From the results of the comprehensive imaging with different tools, we generate a state diagram that defines the qualitative and quantitative aspects of self-assembled, Langmuir films of QDs versus solution concentration and deposition volume. The outcome is a statement of the optimal concentrations and deposition volumes to deposit QDs as Langmuir films and thereby obtain consistent, uniform, well-ordered layers. The subsequent application is to improve the quality of coatings that can be formed using either LS or Langmuir-Blodgett methods.

EFFECTS OF SOLVENT VARIATION TO FUNCTIONALIZE GLASS WITH CHLOROTRIMETHYLSILANE. *JONATHAN COOKSTON* AND JEFFREY WEIMER, UNIVERSITY OF ALABAMA IN HUNTSVILLE.

We studied the variation of solvent in a known process of functionalizing glass surfaces with chlorotrimethylsilane (CTMS). The characteristics of glass treated with CTMS in toluene were previously documented. We compared the prior results to those using green and biocompatible alternatives ethyl acetate and acetonitrile. Contact angles of water droplets on the surfaces of these glass surfaces were measured using a Ramé-Hart goniometer. The values were related to uptake of CTMS on the surface. Uptake curves of coverage versus concentration were measured. Results suggest no significant difference occurs using different solvents. Storage of CTMS in acetonitrile solutions underwent chemical reactions to form crystal products.

CYCLIC ASYMMETRIC ALDOL ADDITIONS AND DEHYDRATIONS IN HOT PRESSURIZED WATER. *OLIVIA DEN BESTEN* AND JOHN BERCH, HUNTINGDON COLLEGE.

Green adaptations to known asymmetric aldol additions were investigated by replacing standard organic solvents with acidic, basic, and neutral Hot-Pressurized Water. Spontaneous dehydrations to the enone were observed using proline as the chiral catalyst; however, stereoselectivity was very low. Given the hydrophilic nature of proline, more hydrophobic amino acids were tested. N-boc Alanine was evaluated as a catalyst in an attempt to mimic the secondary amine properties of proline. Significant increases in stereoselectivity and overall yields of alcohol and enone mixed products were observed.

GREEN MODIFICATIONS TO THE HAJOS PATHWAY TO AN IMPORTANT STEROID INTERMEDIATE. *CAROLINE COOPER* AND JOHN BERCH, HUNTINGDON COLLEGE.

Green modifications to the Hajos pathway to the Wieland-Miescher ketone where investigated. Special emphasis was given to the second step, synthesis of the alcohol, and third step, synthesis of the enone product, with goals of increasing stereoselectivity in hot pressurized water. Given the hydrophilic nature of proline, more hydrophobic amino acids were tested. Lastly, to mimic the secondary amine properties of proline, N-boc Isoleucine was evaluated. Both changes lead to significant increases in stereoselectivity and overall yields of alcohol and enone mixed products.