2017 Belmont Undergraduate Research Symposium

Chemistry

Moderator: Alison Parker, Ph. D.

April 20, 2017, 3:45-5 p.m.
JAC 5004

3:45-4:15 pm

Greening the Synthesis of Virstatin: Finding an Alternative Solvent to Dimethylformamide

Morgan McCauley
Faculty Advisor: Kimberlee Entsminger, Ph.D.

Vibrio cholerae, the causative agent of two of the seven recorded cholera pandemics, is a facultative anaerobic, gram negative bacteria. The main pathogenic effect is life-threatening acute diarrhea that cannot be helped by rehydration or electrolyte therapy. The most common treatment of cholera, like many other bacteria, is through the administration of antibiotics. *Vibrio cholerae*, like many bacteria, is developing a resistance to classic antibiotic treatments, which is why the innovation of new treatments is necessary. Virstatin is a compound that takes a new route to treating V. cholerae by inhibiting ToxT, a transcription regulator. The synthesis of virstatin is completed in two steps. The first step of the reaction is a Gabriel synthesis that uses dimethyl formamide (DMF) as its solvent. DMF is a toxic solvent that does not have any known replacements in reactions like the one being performed. The goal of the current experiment is to green the synthesis of virstatin by discovering a satisfactory benign alternative solvent to DMF. Three solvents were tested for applicability: DMC (dimethyl carbonate), CPME (cyclopentyl methyl ether), and ethanol. Purity of product and reflux time were taken into account to determine the applicability of each solvent. The purity of the product was determined by NMR, IR, and melting point. The reaction was followed by TLC (1:1 ethyl acetate: hexane).

4:15-4:30 pm

Exploring Computation Chemistry Techniques with a Copper Complex

Emily Cottingham
Justin J. Stace, Ph.D.

Computational Chemistry techniques can be used to verify experimental data from research. Here a proposed mechanism from a copper complex was studied to attempt to determine various intermediates that could be present in the reaction. CP2K, with its free, open-source code, is a powerful computational tool that can be utilized to analyze real and hypothetical molecules to determine various quantum chemistry calculations including vibrational energy, bond energy, and optimal bond length. The CP2K software is primarily used with the purpose of educating undergraduate Chemistry students on the basic ideas of Computational Chemistry. In this study, the CP2K software is applied to determine physical parameters of a hypothetical copper square-

planar nitrogen molecule similar to a series of complexes under study in our laboratory. The results of the computational work shows the limits of the software for actual research work instead of as a learning tool for undergraduate work.

4:30-4:45 pm

Synthesis, Characterization, and Unusual Solvation and Luminescent Properties of Terbium Amine Complexes

Libby Ligon
Faculty Advisor: Justin Stace, Ph.D.

Synthesized trivalent lanthanide ion-amine complexes exhibit unique properties and have potential for application in biological-mimic catalysis, photocatalysis, and photoluminescence. Here, three terbium-amine complexes have been synthesized by the reaction of terbium(III) nitrate with 13daprop (1,3-diaminopropane), 15dapent (1,5-diaminopentane), and phen (1,10-phenanthroline) in methanol. The off-white product of each reaction precipitates at -20°C overnight and is captured *via* filtration. All three complexes form colloidal suspensions in water and acetonitrile. The colloidal suspensions strongly absorb ultraviolet radiation. The $Tb(phen)_2$ complex also exhibits very strong visible luminescence, and fluorescence lifetime data for $Tb(phen)_2$ reveals a relatively long-lasting luminescence (~0.4 ms). Results from elemental analysis leads to speculation that the Tb(13daprop) and Tb(15dapent) complexes are polymers. The photophysics of $Tb(phen)_2$ are discussed in detail.

4:45-5:00 pm

Cavity Ring-down Spectroscopy

Bailey Rose
Faculty Advisor: Thom Spence, Ph.D.

Cavity ring-down spectroscopy is an ultrasensitive direct absorption technique that has been, for the most part, only applied to absorbers in the gas phase. Here, a cavity ring-down system has been built using a nitrogen pumped dye laser, and a decay signal has been acquired. An electrospray ionization (ESI) source will be used to produce gas-phase ions from the condensed phase for detection via cavity ring-down spectroscopy. With this technique, ions separated by traditional chromatographic techniques can be detected at significantly lower concentrations than by performing absorption spectroscopy on the condensed phase analyte.