### 22<sup>nd</sup> Annual Natural Sciences Academic Festival Chemistry Department Capstone Presentations *Friday*, 6 May 2016, Rieke 103

#### 1:45 PM Thomas Kolibaba

# Investigation of the phase behavior of a novel diblock copolymer electrolyte system with potential applications in lithium-ion batteries by atomic force microscopy

Solid polymer electrolytes offer the possibility of combatting some of the safety issues inherent in current lithium-ion batteries. However, in current polymer electrolytes, ionic conductivity is directly tied to segmental rearrangement of the polymer backbone. A variety of novel oligo(ethylene oxide) grafted diblock copolymers with bulky backbones were synthesized from basic building blocks and characterized for use as solid polymer electrolytes which can decouple ionic conductivity from local segmental dynamics. The phase behavior of these systems was studied by atomic force microscopy and appears to deviate substantially from standard theoretical random coil – random coil diblock systems. This deviation is believed to be due to a conformational asymmetry in the two blocks studied this system, with this effect seeming to be exaggerated as the oligo(ethylene oxide) sidechain lengths increase.

2:30 PM - 3:30 PM Poster Presentation Session Snack Buffet Morken Center Atrium/Hallway

#### 3:40 PM Brock Lynde

# Release of provitamin D and other substituted 1,3-cyclohexadienes by a retro-nitroso-Diels-Alder reaction: a diene structure-kinetics study.

The retro-Diels-Alder reaction is a potential method for the slow, controlled release of diene molecular cargo from a polymeric carrier. In this study, 1,3-cyclohexadiene and three other substituted variants were chosen to probe the effects of diene structure on retro-nitroso-Diels-Alder reactions. Specifically, the natural products 7- dehydrocholesterol (provitamin D3), ergosterol (provitamin D2), and αterpinene were selected due to their variations in cyclohexadiene substitution and the potential application of vitamin-polymer conjugates. Nitroso-Diels-Alder adducts of the four dienes were synthesized by reaction with N-p-nitrophenyl-N'-nitrosocarbamide (generated in situ by oxidation of the corresponding hydroxyurea) under anhydrous conditions at ambient temperature or below. When these Diels-Alder adducts are heated under aqueous conditions, they undergo retrocycloaddtion to free the diene "cargo". The released nitroso dienophile hydrolyzes rapidly to produce 4-nitroaniline, nitroxyl (H-N=O), and carbon dioxide (CO2). The rate studies for the decomposition were carried out by warming our model compounds in aqueous 1,4-dioxane at temperatures between 37-50 °C and monitoring by UV-visible spectroscopy. Multicomponent spectrophotometric analysis and psuedo-first-order kinetics modeling were performed on the spectroscopic data by utilizing the steady-state approximation. An Arrhenius plot was used to deduce the activation energy for the rate-determining retro-Diels-Alder reaction step in the mechanistic model.

4:30 PM

Keynote Speaker:

Bessie A. Young, MD/MPH, PLU '83

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