Department of Chemistry Seminar

“Supramolecular assembly and structural trends within a three part series of rare-earth p-halobenzoic acid-terpyridine hybrid materials”

The study of f-element materials assembled through covalent means is a rich area of structural chemistry with fundamental and technological aspirations for applications in luminescent and magnetic materials. The addition of supramolecular interactions as a means to assemble f-element materials, however, remains underexplored and offers possibilities of elucidating new structure-property relationships. Moreover, the ‘rules’ guiding assembly criteria have not been established. We have committed to a comprehensive, explorative synthesis effort to evaluate new 4f-materials with supramolecular interactions of interest. As such, sixty rare-earth (La3+-Lu3+, Y3+) p-halobenzoic acid-2,2’:6’2”-terpyridine complexes have been hydrothermally synthesized at varying temperatures and structurally characterized by single crystal and powder X-ray diffraction. These sixty structures are all part of three separate series of materials, where all reaction conditions were kept constant, except for the systematic variation of the halogen atom (chlorine, bromine, and iodine) on the benzoic acid ligand. Fifteen compounds contain p-chlorobenzoic acid (synthesized by Korey Carter), twenty-four have the p-bromo- analogue, and the remaining twenty-one contain p-iodobenzoic acid. All structures are binuclear (or pseudo-binuclear) species with only slight differences in coordination environment. They all contain ‘capping’ terpyridine ligands, which afford control over building unit speciation, and halogen-functionalized benzoic acid ligands, providing peripheral halogen atoms for halogen-based supramolecular assembly. Non-covalent interactions observed include: halogen-halogen, halogen-π, and π-stacking interactions. Despite the broad similarities between the six structure types within all sixty compounds, an evolution of the coordination environment of the RE3+ metals is observed. The relative strength of halogen-based supramolecular interactions, using the crystallographic metric of interaction distances, was also explored across the three halogen varied series. Sensitized solid-state visible and near-IR luminescence spectra were also collected and characteristic emission was observed.

BIO
August received his BS degree in Chemistry and History from Dickinson College in Carlisle, PA studying the effects of ultrasound on enzymatic activity and early North American colonial conflict through Col. Benjamin Church. His current research under Dr. Christopher L. Cahill includes crystallography and f-element hybrid materials chemistry.

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Friday, October 7, 2016
SEH B1220
2:00 - 3:00 p.m.
Refreshments will be served at 1:45 p.m.