

## Elizabeth T. Papish

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### Current Research

The main focus of research in my lab has been **bioinorganic chemistry**, but we have recently started a project in **organometallic chemistry** (see below). We are interested in catalysis using new chelates capable of providing N, O and C donor atoms to transition metals and we take our inspiration from both natural catalysts (enzymes) and man-made catalysis.

### Bioinorganic Chemistry

We are interested in making new ligands and complexes to mimic the structure and function of important metalloenzymes. Bioinorganic chemists have gotten very good at modeling the primary coordination sphere of metalloenzymes, but few examples mimic the secondary coordination sphere and thus water-soluble ligands and fast catalysis of hydrolysis reactions have been rare. *This gap in the knowledge base is a problem because it prevents a full understanding of the role that the secondary coordination sphere plays in metalloenzyme function.* We are interested in modeling phosphotriesterase (PTE) since it catalyzes the hydrolysis of both pesticides and nerve gases. Our approach is novel, in that we use triazole based ligands where nitrogen atoms enhance the water solubility through hydrogen bonding, rather than charged groups. Triazole based ligands are hydrophilic and have a propensity for hydrogen bonding interactions that make them well suited for modeling non covalent interactions in metalloenzymes. We are the first group to use sterically demanding tris(triazolyl)borate ligands for transition metal complexes. Furthermore we plan to explore the effect of hydrogen bonding in the vicinity of the metal. It is anticipated that this could stabilize unusual structures. This may lead to novel reactivity since hydrogen bonding, improved water-solubility, and sterically bulky ligands have not yet been combined to form low coordinate complexes with biologically relevant metals. These ligands, complexes, and any resulting catalysts could have a big impact due to their relevance to metalloenzymes and the potential for green chemistry applications. The scope of potential research applications is large and includes modeling various esterases, carbonic anhydrase and oxygenases. Tris(triazolyl)borate complexes are structurally very similar to the corresponding tris(pyrazolyl)borate complexes, but should contain a more electrophilic metal center that may be ideal for Lewis acid catalysis in environmentally friendly solvents.

### Organometallic Chemistry

N-Heterocyclic carbene (NHC) ligands have the potential to replace phosphines in many catalytic processes. They could make important organic transformations such as C-H activation, C-C coupling, and ionic and transfer hydrogenations greener, more robust and more efficient. Very few sterically bulky chelating carbene ligands have been synthesized, and thus low coordination numbers have rarely been achieved with chelates. We plan to use bulky imidazole and water-soluble triazole rings to design novel bidentate and tridentate carbene ligands. These ligands will be complexed with late transition metals and the resulting structures will be determined by NMR, IR, and UV-Vis spectroscopies and single crystal x-ray



diffraction. Then we will test for stoichiometric or catalytic hydrogenation of polar double bonds and perform kinetic studies to elucidate the mechanism of new reactions. Our neutral NHC ligands will be unique in their ability to 1) create three metal-carbon bonds with a geometry similar to tris(pyrazolyl)borate complexes, 2) allow the formation of coordinatively unsaturated, highly active metal centers, and 3) allow electronic modification through triazole based carbenes. Additionally, our tripodal carbene ligands will be the first to use a compact C anchor and this will offer advantages in terms of acid stability and charge neutrality that allows the analogy between phosphines and carbenes to be used in catalyst design. These qualities will allow our ligands and complexes to be used in a broad range of organometallic catalysis applications. This research is supported by ACS-PRF (a type AC award in 2008).

### Student Learning Outcomes

Over the past five years, I have had 17 students (mostly undergraduates) and one postdoc working with me on these projects. Students in my group have gained hands on experience in organic synthesis, inorganic synthesis, handling air sensitive materials, various forms of spectroscopy, and reactivity studies for mechanistic experiments. But more importantly, they learned how to design control experiments and ask the sorts of questions that would allow new chemical information to be discovered. I try to help students learn for themselves how to think critically and solve problems.

### Recent Selected Publications

- (1) Gardner, S. R.; Papish, E. T.; Monillas, W. H.; Yap, G. P. A. *Journal of Inorganic Biochemistry* **2008**, in press.
- (2) Papish, E. T.; Donahue, T. M.; Wells, K. R.; Yap, G. P. A. *Dalton Trans.*, **2008**, 2923-2925.
- (3) Jernigan, F. E.; Sieracki, N. A.; Taylor, M. T.; Jenkins, A. S.; Engel, S. E.; Rowe, B. W.; Jové, F. A.; Yap, G. P. A.; Papish, E. T.; Ferrence, G. M. *Inorg. Chem.* **2007**, *46*, 360-362.
- (4) Papish, E. T.; Taylor, M. T.; Jernigan, F. E.; Rodig, M. J.; Shawhan, R. R.; Yap, G. P. A.; Jové, F. A. *Inorganic Chemistry* **2006**, *45*, 2242-2250.