Organometallic Chemistry for Drug and Catalyst Design Jared Pienkos-URP 2025

Tuning the properties of transition metal compound with the N-oxide functional group

Our group is interested in exploiting transition metal compounds as imaging agents to monitor hypoxia, low oxygen concentration, in tumor cells. To do this, we are designing compounds that undergo structural changes in low oxygen concentrations. Past work done by Knox et al. (DOI: 10.1038/s41467-017-01951-0) showed organic dye molecules with a

nitrogen-oxygen bond (*N*-oxide functional group) can be modified by CYP450 enzymes *in vivo* to generate a new species with differing optical properties, which was utilized to monitor hypoxia. Our strategy builds upon this idea but utilizes transition metal compounds containing this *N*-oxide functional group.

For this research, students will synthesize an *N*-oxide containing transition metal compound to determine how the *N*-oxide impacts the properties of the compound. Students will also learn how to model the optical properties of these compounds using computational chemistry.

Synthesis of Trans-bidentate Ligands (Collaboration with Dr. Lee)

Trans-bidentate ligands, which force metals to adapt to a constrained geometry, are useful in the field of catalysis. Our group is interested in synthesizing these types of ligands by exploiting 2-ethynylpyridine bound to square planar or octahedral metal centers in the *cis*-fashion or by modifying halogenated heterocycles using the Sonogashira cross-coupling reaction.

Carbon Monoxide Releasing Molecules

Carbon monoxide (CO) when ingested in large quantities is fatal, however, controlled absorption has shown medicinal benefits. For instance, administration of CO (200 ppm) through the lungs as a mixture with air can decrease inflammation. The drawback of this treatment is that CO is administered globally and can affect areas other than those intended for treatment. A strategy to precisely control the delivery of CO involves binding CO to a carrier molecule, which, when delivered to targeted cells, can be triggered to release CO. Transition metals, because of their affinity for CO, are good candidates for these delivery systems and have been used as CO releasing molecules (CORMs). This project aims to synthesize and study new classes of CORMs.





