

# Rhenium(I) Carbonyl Complexes: Applications in Full-Color Displays

Sibrina N. Collins, PhD

Department of Chemistry, The College of Wooster, Wooster, Ohio 44691

Corresponding Email: [scollins@wooster.edu](mailto:scollins@wooster.edu)

## Introduction

The development of metal complexes as phosphorescent emitters for organic light emitting devices (OLEDs) remains a strong area of interest. Such devices are potentially useful for large flat panel displays. Platinum(II), ruthenium(II) and iridium(III) complexes have been widely investigated as electrophosphorescent materials for OLEDs. However, recent reports have focused on neutral rhenium(I) complexes. In addition, some rhenium(I) organometallic complexes have successfully been incorporated into such devices. These complexes are thermally robust, exhibit high quantum yields at room temperature and short excited state lifetimes. An example of a rhenium(I) organometallic complex,  $\text{Re}(\text{CO})_3(\text{bab})$  (**1**) containing a tridentate ligand ( $\text{N}^{\wedge}\text{C}^{\wedge}\text{N}$ ) is shown in Figure 1.

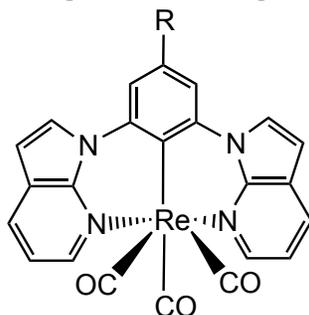
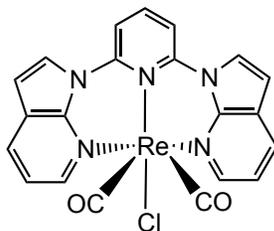


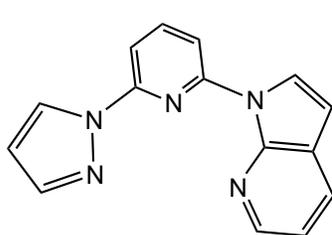
Figure 1. Structure of the  $\text{Re}(\text{CO})_3(\text{bab})$  (**1**) Complex.

Our goal is to use related 7-azaindole ( $\text{N}^{\wedge}\text{N}^{\wedge}\text{N}$ ) ligands for the development of new rhenium(I) organometallic complexes. An example of a new Re(I) organometallic complex,  $\text{Re}(\text{CO})_2\text{Cl}(\text{bap})$  (**2**) is shown in Figure 2. Specifically, we want to compare the  $\text{N}^{\wedge}\text{C}^{\wedge}\text{N}$  ligands with our  $\text{N}^{\wedge}\text{N}^{\wedge}\text{N}$  ligands. *How will changing the coordination environment of the rhenium(I) metal center effect the emission properties?*

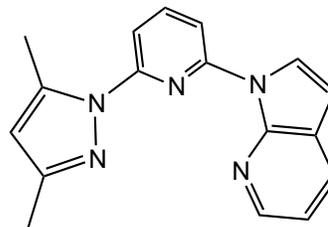
**Preliminary Results.** We recently obtained a grant from the Ohio Super Computer (OSC) in order to predict the properties of our metal complexes before they are synthesized in the laboratory. The geometry optimizations of **1** and **2** were recently completed in our laboratories. The computational predictions of **1** are in good agreement with the literature. Our  $\text{N}^{\wedge}\text{N}^{\wedge}\text{N}$  ligands, specifically pap and dap are prepared through copper-mediated cross-coupling reactions using copper iodide and racemic *trans*-1,2-cyclohexane. Last summer, we successfully obtained an X-ray quality crystal structure of a key synthetic intermediate for our reactions.



**[Re(CO)<sub>2</sub>Cl(bap)] (2; bap = 2,6-bis(azaindole)pyridine)**



**2-pyrazyl-6(azaindole)pyridine (pap)**



**3,5-dimethyl-2-pyrazyl-6(azaindole)pyridine (dap)**

Figure 2. Structures of [Re(CO)<sub>2</sub>Cl(bap)] (2) and pap and dap.

This summer research project entails the synthesis, characterization and computational analysis of the rhenium(I) organometallic complexes, namely **1** and **2** and organic molecules such as pap and dap. Additional tridentate ligands containing N<sup>X</sup>N (X = S, O, and etc) will also be investigated. Computational chemistry will be utilized to predict the properties of the new rhenium(I) complexes that are coordinated to pap and dap.