

Water Soluble Picolamidine Metal Complexes

R Castañeda¹, M Petronis², T Timofeeva³

¹New Mexico Highlands University ²New Mexico Highlands University, ³Chemistry Dept. New Mexico Highlands University

lcast029@uottawa.ca

Water-soluble complexes are attractive in many fields including but not limited to water splitting, polymer catalysis, and MRI contrast agents. In this work picolinamidine (PiAm; Chart 1) was used to build six different water-soluble complexes (1-6; Chart 1) with copper, nickel and zinc and they were studied by X-ray single crystal diffraction, IR, UV-vis, and PXRD. Amidine ligands in general had not extensively been used in coordination chemistry, and PiAm has a great potential to build water-soluble complexes as the amidine group is capable to act both as hydrogen bond donor and acceptor. By design it is possible to control the number of ligands coordinated to individual metal ions, for example 1 and 2 (Chart 1) have only one ligand coordinated while 3-6 (Chart 1) have two PiAm ligands coordinated to the metal ions. Complexes 1 and 2 are very similar with the main difference being the substitution of one chlorine atom for one bromine atom. Unsurprisingly these complexes are isomorphous with the monoclinic P21/n space group and a minor increase of 4.5% of the total unit cell volume for 2 due to the change of chlorine for bromine. Complexes 3, 4, and 5 share a similar framework with the metal ion located at an inversion center, resulting in the same ligands opposite to each other, in an octahedral cis configuration. Despite the similarities between 3 and 4, only one single crystalline phase was found for 3, whereas two different polymorphic structures were found in the case of 4 (4a and 4b). Both 4a and 4b have the monoclinic P21/n space group and 4a is isomorphous to 3. The differences in coordination of these complexes along the differences in hydrogen bonding and crystal packing will be discussed in this work. In conclusion, PiAm was successfully used to synthesize six different complexes with remarkable water solubility and stability and further studies will be underway for the copper complexes to measure their activity as MRI contrast agents.

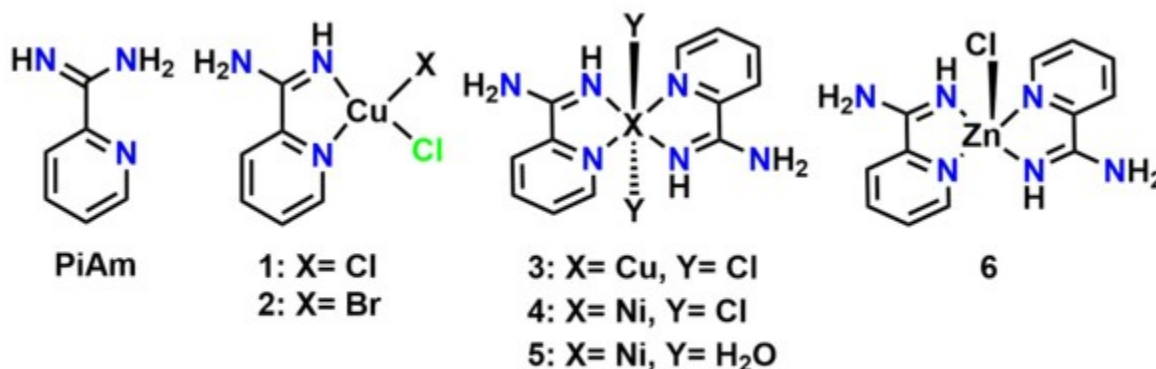


Chart 1. List of amidine complexes recently synthesized at NMHU.

Figure 1