Utilizing Copper Complexes of the Ligands (2-aminoethyl)bis(2-pyridylmethyl)amine and N,N-bis(2-pyridylmethyl)aminobutanol as Catalysts in ATRA Reactions

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Atom Transfer Radical Addition (ATRA) is an organic reaction that functionalizes olefins. Products from this reaction can be used to make important starting reagents. The goal of this project was to design new catalysts that efficiently facilitate ATRA. Currently, the most active catalyst used in ATRA incorporates a tripodal design. This configuration can lead to structural crowding of the active site during catalysis, reducing the efficiency of the reaction. We hypothesized that developing a catalyst that alleviates this structural issue, by increasing access to the active site, could result in increased efficiency, conversion, product yield, and turnover frequency. Two catalysts were synthesized that maintained the important tripodal motif while reducing crowding by modifying its ligand structure. The ligands (2-aminoethyl)bis(2-pyridylmethyl)amine and N,N-bis(2-pyridylmethyl) aminobutanol were synthesized and analyzed using various spectroscopy techniques to confirm their structure. The ligands were reacted with copper bromide to generate our desired catalysts. Catalyst structures were confirmed with spectroscopy techniques and single-crystal X-ray diffraction. ATRA reactions were performed using our catalyst and various olefins (alpha-olefins, aromatic-olefins, and branched olefins incorporating terminal C=C functional groups).Proton NMR spectroscopy was used to measure catalyst activity at various concentrations and results were compared to known catalysts. Results indicate that catalysts made with N,N-bis(2-pyridylmethyl) aminobutanol produced better yields when compared to catalysts made with (2-aminoethyl)bis(2-pyridylmethyl)amine. These results showed that mixed-donor catalysts perform more effectively when compared to same-donor catalysts. Compared to known catalysts, our catalysts made with N,N-bis(2-pyridylmethyl) aminobutanol were more efficient when using alpha olefins compared to aromatic or branched olefins.