

Greening the Synthesis of Cp*Co Catalyst Complexes

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Catalysts, molecules that speed up the rates of chemical reactions, are essential for the production of countless consumer goods. Cobalt catalysts in particular are highly sought after for their use in the synthesis of soaps, shampoos, plasticizers, and lubricants. Cobalt catalysts are highly customizable and can be tailored to suit the needs of a reaction. The customization process for the catalysts synthesized in our lab starts with a cobalt bis alkene complex such as pentamethylcyclopentadienyl cobalt bis-ethene (referred to as Cp*Co(C₂H₄)₂, or simply bis-ethene). These molecules serve as templates for the production of future cobalt catalysts.

In the summer of 2023, my research primarily focused on improving the synthesis of bis-ethene. This was accomplished through the use of UV light as a mechanism to promote ligand substitution. In all, the new photochemical procedure eliminated 4-5 days of synthetic work and the use of toxic, heavy metal reagents. This summer I was able to build on my findings and continued to optimize the synthesis of bis-ethene while simultaneously pursuing the use of UV light to coordinate various new alkene ligands, creating new Cp*Co catalyst complexes.

To further optimize the synthesis of bis-ethene, I focused on manipulating the conditions of the reaction, such as time, temperature, and concentration. Currently, the photochemical procedure works best at low concentrations of starting material (< 0.01 mM). Thus, an investigation into higher concentrations is necessary in order to create a more useful synthetic route. However, reactions with higher concentrations of starting material (0.04 mM <) posed issues with the synthesis. At higher concentrations, a dark green impurity formed in the solution, which is a result of the starting material reacting with itself and forming a dimer. Although the intensity of the green solution may point toward the idea that the dimer is the major product of the reaction, column chromatography paired with H¹-NMR analysis indicates that the major product is still the desired bis-ethene, but followed closely behind by unreacted starting material.

I manipulated the time and temperature of the reaction at various concentrations and compared the quantitative ratio between final product and starting material between reactions to identify which conditions may have the biggest effect on increasing the yield of the reaction. So far, lengthening the time of irradiation appears to have the biggest effect on reducing the amount of starting material. I hypothesized that running the reaction at cold temperatures (-78° C) would decrease dimerization, but experimental evidence proved otherwise, as dark green was still observed.

Expanding from ethene, photochemical coordinations of 2,5-norbornadiene, 1,4-cyclohexadiene, and cyclooctatetraene were tested and analyzed with H¹-NMR, giving evidence of coordination and formation of a cobalt catalyst complex. Additionally, a past coordination of 1,5-cyclooctadiene was structurally characterized via X-ray diffraction.

In the future, I would like to continue to increase the length of irradiation to test whether the dimerization product has a half-life in solution and can be circumvented with time. Additionally, I would like to continue to grow x-ray quality crystals to structurally characterize more unique cobalt catalyst complexes.

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