

Synthesis of Cobalt Complexes through Photochemistry

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The production of linear α -olefins (LAOs) has grown into a multi-billion-dollar industry as they have become an integral organic compound (carbon-containing molecule) for a variety of industries. These compounds are used to manufacture high-demand products like detergents, lubricants, plasticizers, and soaps. The structure appears very simple; however, the production is complicated.

The current commercial production of LAOs is inefficient as it is environmentally harmful and expensive. In addition, branched α -olefins are a common byproduct as they are more thermodynamically stable than LAOs. Unfortunately, these compounds are not useful commercially and are discarded as waste. The current synthetic route used for the formation of LAOs involves metals like zinc and mercury. The use of these toxic metals and the mass waste produced create additional health and environmental issues, which can be detrimental when these compounds are mass-produced since their existence is necessary for multiple industries. As a result, an effective, alternative method to control the ratio of linear to branched products through the dimerization of shorter LAOs. The Broene lab aims to use cobalt to synthesize an eco-friendly, highly efficient catalyst that speeds up the rates of chemical reactions and can accomplish the dimerization of LAOs.

My research investigates the synthesis of the ligand 8-quinolyl-tetramethylcyclopentadienyl and its precursors. The steric interactions of this previously synthesized tailored ligand is measured by the three-dimensional cone angle created by the metal center and the outermost edge of the ligand's atoms. The decreased steric interactions of this molecule allow for the manipulation of the ratio of linear to branched products as this ligand binds in a way that favors the formation of LAOs. I specifically focused on synthesizing the 8-quinolyl-tetramethylcyclopentadienyl precursor more efficiently.

To accomplish this, I began by scaling up the preparation of 8-bromoquinoline, a necessary starting material in the next synthesis step of this ligand. I investigated two different reaction schemes for the preparation of 2,3,4,5-tetramethyl-1-(8-quinolyl)cyclopentadiene, which is another necessary precursor, to determine the most efficient protocol. I also manipulated the purification process to improve the yield. I was able to increase the scale of this reaction efficiently. The coordination of this ligand with the dicobalt octacarbonyl was attempted.

The materials synthesized will be a necessary part of my Honors project this fall where I will focus on photochemically – involving the use of heat and light – synthesizing the desired cobalt catalyst. The carbonyl (CO) bonds on cyclopentadienyl dicarbonyl cobalt (I) species have been demonstrated to be photochemically sensitive, so the irradiation of tetramethylcyclopentadienyl quinoline dicarbonyl cobalt (I) with ultraviolet light is expected to photochemically displace the carbonyl group. Ideally, the nitrogen of the quinoline will remain preventing the rotation of that section of the ligand, eliminating the cone angle entirely, leaving a 2D structure favoring the formation of LAOs. Moreover, the application of this catalyst under varying conditions for the dimerization of LAOs must be studied further, so that the ratio of desired α -olefins can be maximized.

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