# Ligand Precursors for Linear Alpha Olefin Dimerization with Cobalt Catalysts

#### Katie Rea, 2025

The production of linear  $\alpha$ -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 synthetic oils, surfactants, and are co-monomers in an assortment of plastic compounds (Forestiere & Oliver-Bourbigou, 2009; Ittel, 2000; Lappin, 1989). The structure appears very simple; however, the production is complicated, often producing more waste than desired materials.

LAOs are produced commercially; however, the production results in many other undesired products and involve the use of metals like zinc and mercury (Forestiere & Oliver-Bourbigou, 2009). The use of these toxic metals and the mass waste produced pose health and environmental issues, which can be detrimental when these compounds are mass-produced. As a result, an effective, alternative method to control for the length of LAO is is through the dimerization of shorter linear  $\alpha$ -olefins. The Broene lab aims to use cobalt to synthesize an eco-friendly, highly efficient catalyst that can accomplish the dimerization of LAOs.

My 8-week project focused on the synthesis of ligand precursors for selective LAO dimerization catalysts. A catalyst is a substance that increases the rate at which a reaction occurs, without being consumed in the reaction. In my case the ligand was constrained- which means that it had fewer degrees of freedom compared to unconstrained ligands, and our hypothesis was that as this ligand would present as smaller and therefore more selective for LAO formation. The compounds I handled were often air-sensitive, so most of the summer was spent performing Schlenk line chemistry, which allowed me to control the atmosphere surrounding these air-sensitive compounds often by introducing nitrogen.

I started the summer synthesizing pentamethylcyclopentadiene cobalt bis-ethene (Cp\*Co(ethene)2) which is necessary for coordinating various ligands with cobalt. After a sufficient amount had been synthesized that could be used throughout the summer, I transitioned to synthesizing Cp\*CoI<sub>2</sub>, which had the potential of being utilized as an effective ligand precursor, which was partially demonstrated by previous work (Harris, 2020). Not all attempts at synthesizing this compound were successful, which was shown by data of the molecular structure collected through nuclear magnetic resonance—NMR. In the last week, I purified previously synthesized Cp\*quinoline. The identity of the purified product was confirmed using both NMR spectroscopy and mass spectroscopy, which provide details into the molecular structure and weights of compounds. This compound will be a necessary part of my independent study where I will focus on photochemically—involving the use of heat and light—synthesize a cobalt catalyst, which I plan to conduct in the fall of 2023 in the Broene Lab.

## **Faculty Mentor: Professor Richard Broene**

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