

Greening the Synthesis of Cp* Cobalt Bis Alkene 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.

The current synthetic route for bis-ethene is a 4 step, redundant, multi day process with relatively poor yields. Additionally, the synthesis requires a combination of zinc and mercury, producing toxic and heavy metal waste that should be avoided if possible. A new synthetic route that eliminates time intensive reactions and hazardous reagents is highly desirable.

My research investigates the use of ultraviolet light to directly convert Cp*Co(CO)₂ (an easily obtainable molecule) into bis-ethene, thus eliminating multiple days of synthesis and the use of toxic reagents. I have found that in the presence of excess ethene gas and 254nm light, Cp*Co(CO)₂ is able to substitute an ethylene ligand in place of a carbon monoxide ligand in only 1 hour. One caveat of this procedure is that, so far, I have been constrained by the amount of starting material I can use while still synthesizing the desired bis-ethene product.

I believe that the reaction is bimolecular and requires an excess of ethene with respect to the Cp*Co(CO)₂. At higher concentrations of Cp*Co(CO)₂, a reaction occurs between the starting material and itself, known as a dimerization reaction, to give a product tentatively assigned as a bridging carbonyl species with the formula [Cp*Co(CO)]₂. The dimerized material is an unwanted side product, and cannot be converted into bis-ethene. Thus, finding a way to inhibit the dimerization reaction via increasing the concentration of ethene or reducing the power of the UV light source would be beneficial.

Success with ethene allowed for an extension to other more complicated alkenes, such as 1,3-butadiene and 1,5-cyclooctadiene, to give Cp*Co(butadiene) and Cp*Co(COD). Unlike ethene, which is a gas at standard temperature and pressure, the previously mentioned alkenes are liquids and as the reaction can be carried out in a solution of the alkene itself providing much higher concentrations. This allows for the larger scale production of brand new Cp*Co bis alkene complexes.

In the future, I would like to further investigate ways in which the dimerization reaction can be prevented, especially through the manipulation of the UV light source. Pulsing the UV light over periods of time will allow for the concentration of ethene to increase in the solution again, hopefully preventing the dimerization reaction.

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