



THE REACTION OF PHENYLACETYLENE WITH PINACOLBORANE CATALYZED BY TITANOCENE DICARBONYL

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In modern organic chemistry synthesis, reagents and complexes containing transition metals are important because they allow seemingly impossible reactions to occur easily. The hydroboration of carbonyl compounds is an efficient synthetic route to alcohols, and stoichiometric methods utilize boranes (1-6) to synthesize borates, which are then hydrolyzed to alcohols. The frameworks of Mg, Zn, and Ti perfectly illustrate metal-catalyzed hydroboration reactions that do not use expensive and/or hazardous metals. Likewise, we aim to provide carbonyl hydroboration catalysts based on earth-abundant and low-toxicity metals in a cheaper and more environmentally benign way as opposed to more costly rare-metal systems.

Titanium is an attractive choice in this respect, since it is the fourth most abundant metal in the earth's crust (0.86% by weight) after aluminum, iron and magnesium.⁽⁷⁾ The catalytic process for alkene hydroboration is inverse first order in borane and first order in alkene. This indicates that the reaction occurs by reversible dissociation of borane and coordination of alkene to form an alkene borane complex that undergoes elimination of alkylboronate ester.⁽⁸⁾ Once the vinyl ester is obtained, converting it to a ketone is the final step.

The project's overarching goal is to attempt to make vinyl boronate esters. The process begins with a desired mass of the starting alkene, phenylacetylene. In order for the reaction to proceed, Pinacolborane must be added so that the hydroboration can occur. Next, a catalyst is used in order to speed up the reaction using far less energy. After the reaction has finished, Infrared and Proton NMR spectrums will be analyzed in order to determine where the hydroboration occurred. After conducting multiple trials, assessing the possibility of converting the vinylboronate ester to a ketone through an enol intermediate.