Abstract
Developments of new pharmaceuticals and fuels synthesized from hydrocarbons are currently inefficient due to the large amounts of heat required in order to alter inert carbon-hydrogen bonds. There are an abundance of natural organic hydrocarbon compounds that could be used in this synthesis; however, the current synthetic methods rely heavily on harsh conditions involving strong acids and bases or high-energy inputs in order for the reaction to yield product. Previous studies have demonstrated the possibility of tethering transition metals to the hydrocarbons in order to weaken a carbon-hydrogen bond and replace the hydrogen with a more useful element such as nitrogen, oxygen or sulfur. We have synthesized and characterized a related palladium complex and tested its reactivity with different solvents.

Introduction
A wide variety of products ranging from aspirin to plastics are readily available to consumers through the synthesis of petrochemicals. A product of crude oil and natural gas, petrochemicals are modified hydrocarbons through C-H bond activation, which replaces select hydrogen atoms with a functional group.\(^1\)

\[
\text{Hydrocarbon} \quad \text{Aspirin}
\]

Naturally ubiquitous but inert, C-H bonds are commonly activated through cracking or thermal dehydrogenation requiring both extreme temperatures and lots of energy to overcome high bond energies.\(^1,2\) The increasing use of modified hydrocarbons demands the investigation of new reaction mechanisms that support a more environment-friendly C-H bond activation. One example implements a transition metal tether along with electron withdrawing groups to the starting hydrocarbon compound to cause the targeted C-H bond to become more susceptible to activation.\(^3\)

\[
\text{C-H bond} \quad \xrightarrow{\text{5 mol\% Pd(OAc)}_2} \quad \text{Modified bond}
\]

Our research seeks to study the C-H bond breaking step to further understand these reactions.

Proposal
We propose the synthesis and study of the following metal complex to investigate breaking the C-H bond shown.

\[
\begin{align*}
\text{2-benzylpyridine} & \quad \text{Ligand (L)}_1 \\
\text{N} & \quad \text{Pd-L}_1 \\
\end{align*}
\]

Results and Discussion
The C-H bond is still present at the same position as in Pd-L\(^1\)-NCCH\(_3\); however more noise in the NMR suggests less NCCH\(_3\) bound to the open-site and moving closer to product A. No significant reaction was observed after heat was applied to the reaction for several days.

Conclusion & Future Directions
Several new palladium complexes have been synthesized and observed by NMR spectroscopy. Various functional groups have been shown to bind to palladium, including phosphine (PPh\(_3\)), nitrile (NCCH\(_3\)) and ketone ((CH\(_3\))\(_2\)C=O). NMR data show that initial attempts to break a C-H bond and form a palladium-carbon intermediate under mild reaction conditions have not been successful. Future studies will focus on reactivity of analogous palladium complexes.

References

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