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The Breaking of Carbon-Carbon Bonds in Alkyl Ketones

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Product Selectivity in the C-C Bond Activation of Alkyl Ketones

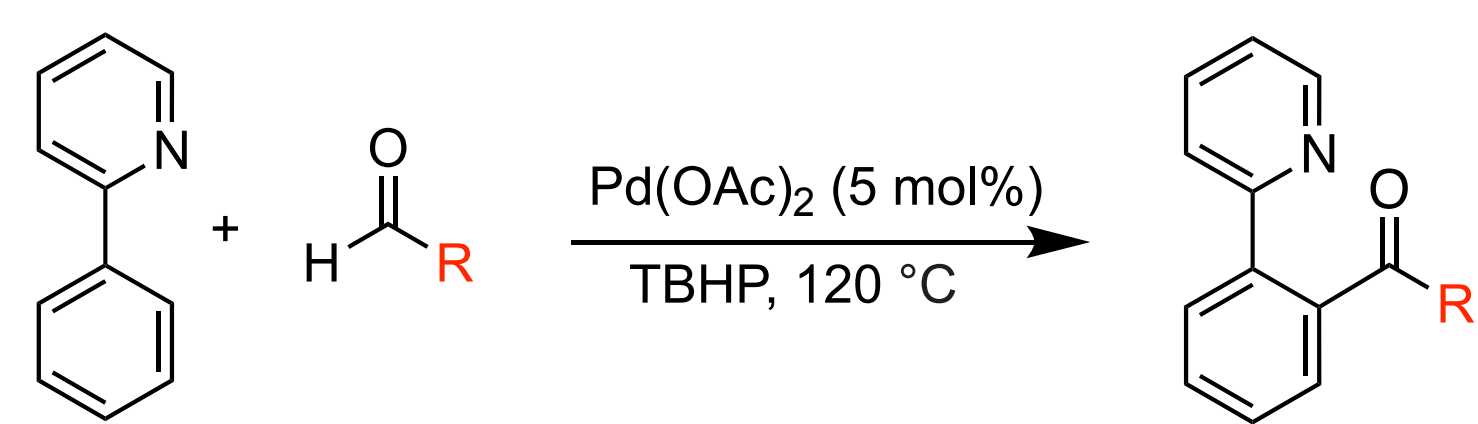
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Abstract

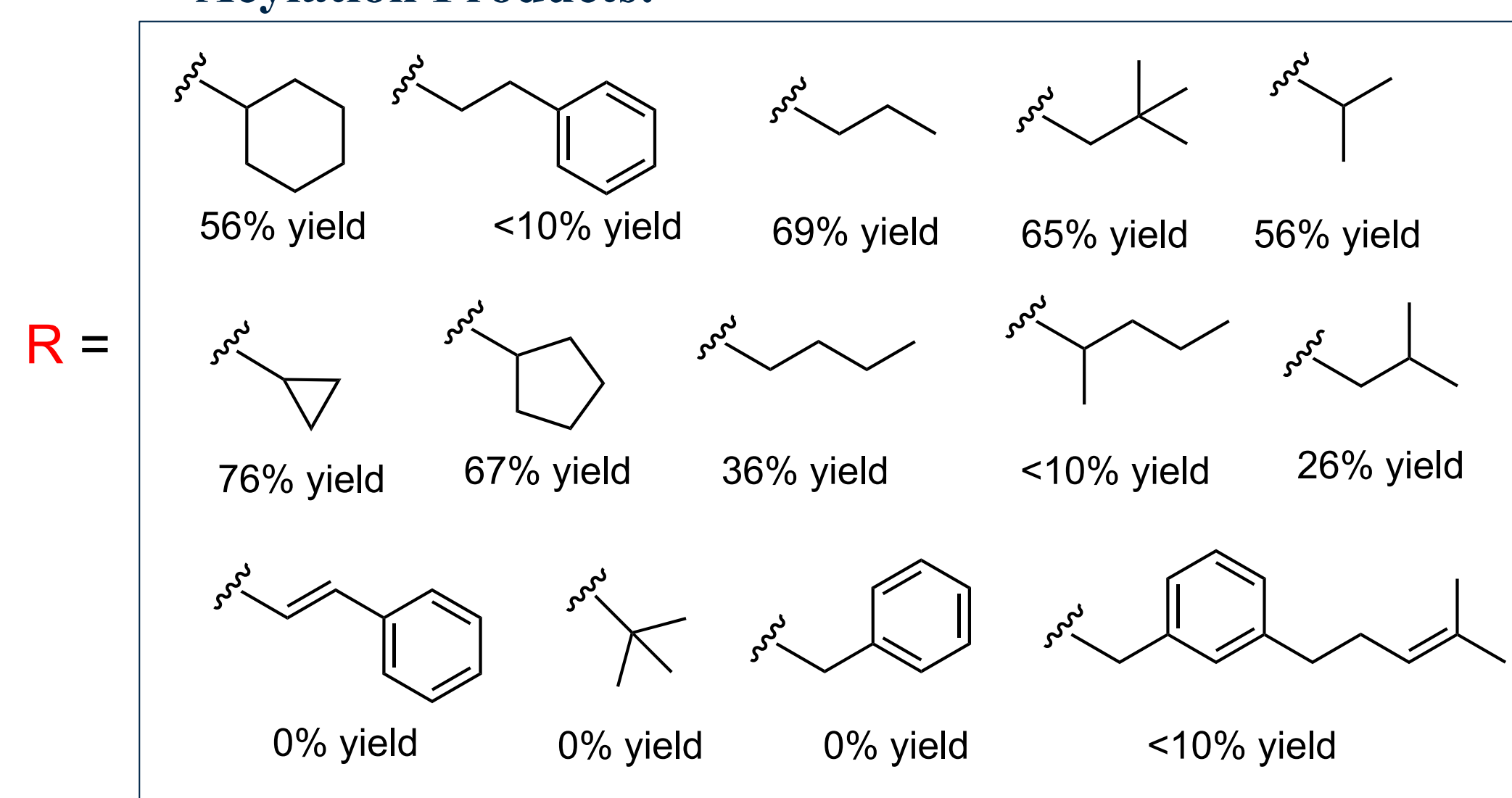
The breaking of carbon-carbon bonds holds great promise for organic chemistry synthesis. This project specifically looks at using a rhodium catalyst to perform a decarbonylation. The focus is to observe the outcome of a variety of different alkyl groups attached to ketones as they undergo decarbonylation reactions. Depending on the alkyl ketone, the reaction can proceed via direct decarbonylation and/or beta-hydride elimination. The goal for this project includes controlling the selectivity of these reactions for the desired product and expanding the library of successful ketones containing alkyl groups used for the reactions.

Acylation for Ketone Formation



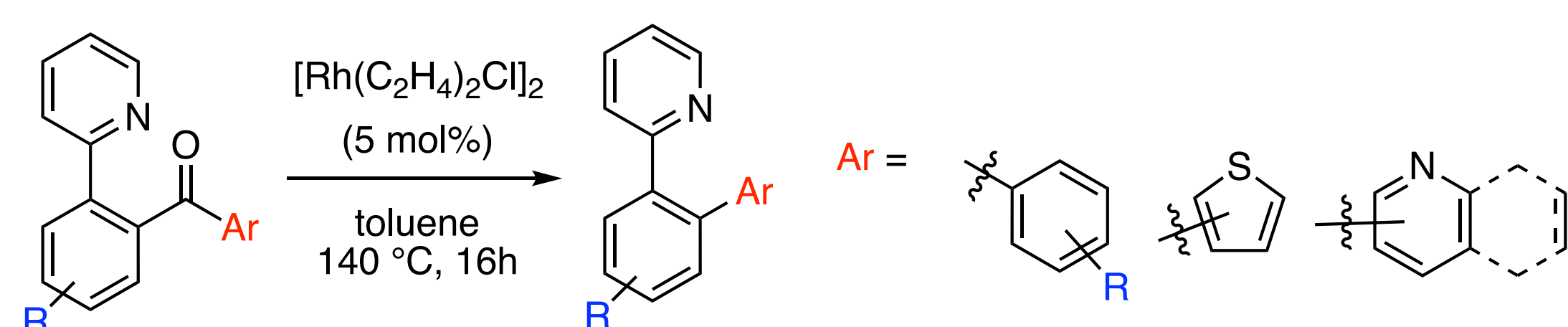
- The ketones formed for the decarbonylation reactions were created through a palladium-catalyzed carbon-hydrogen activation process.

Acylation Products:



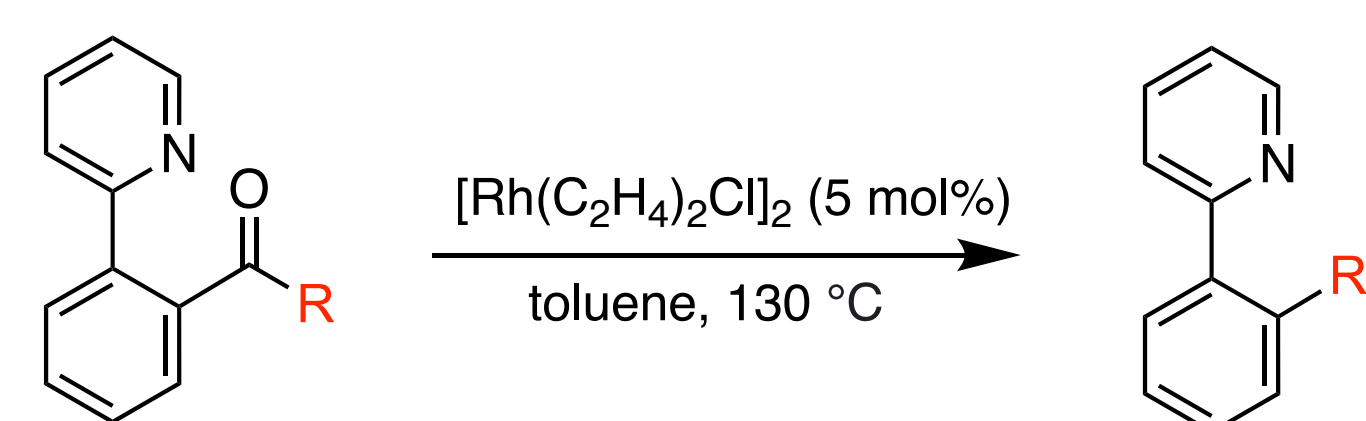
Baslé, B.; Shuai, L. *Adv. Synth. Catal.* **2010**, 352(7), 1145-1149.

Decarbonylation



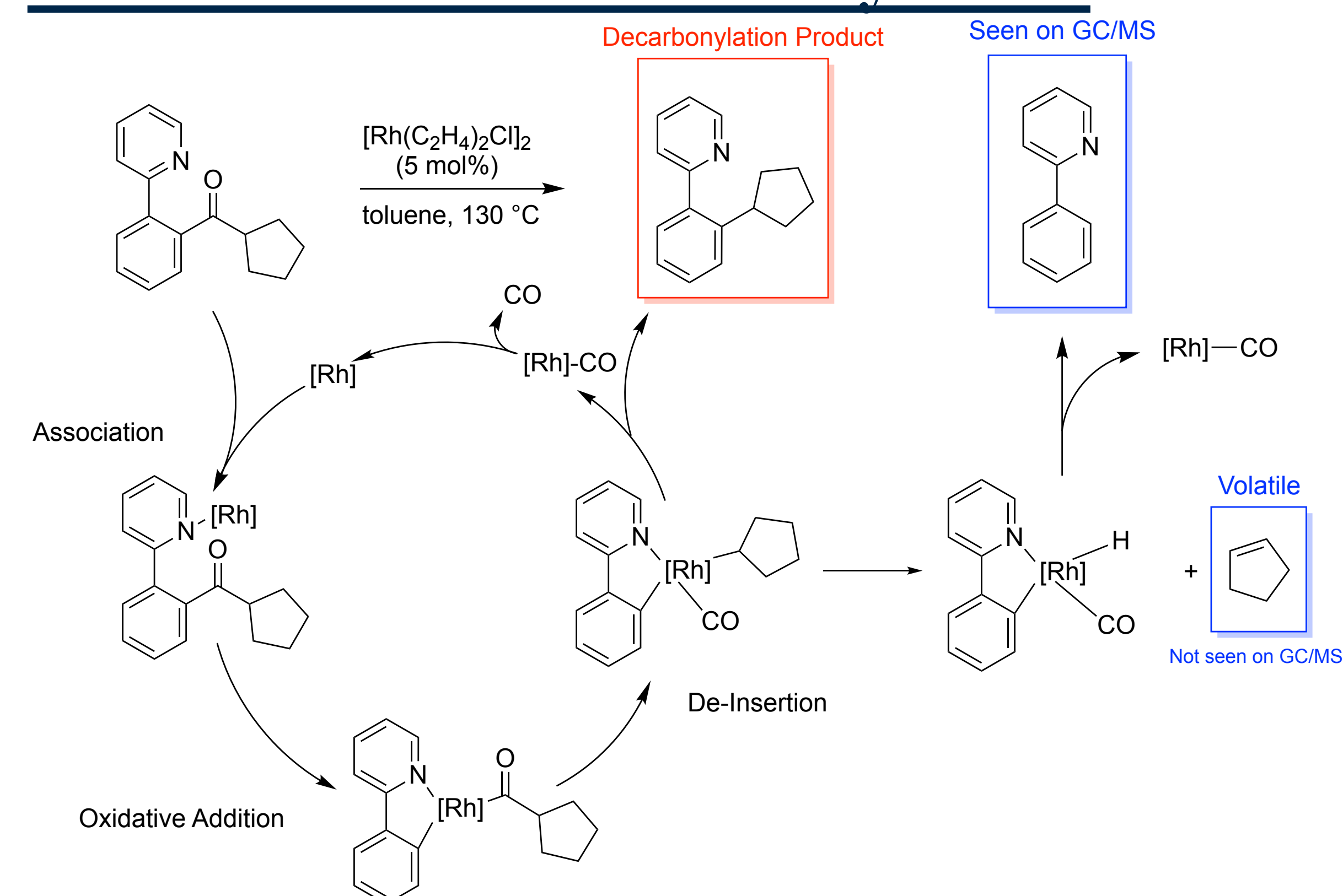
- 29 examples of different aryl groups were previously tested with the decarbonylation reactions with ~73-98% yield.

Lei, Z.; Li, H.; Li, Y.; Zhang, X.; Chen, K.; Wang, X.; Sun, J.; Shi, Z. *Angew. Chem., Int. Ed.* **2012**, 51, 2690.
 Wagner C.; Salisbury E.; Schoonover E.; VanderRoest J.; Johnson J. *Tet. Lett.* **2021**, 73, 153132.



- Due to the high success rates of the aryl groups, exploration of alkyl groups has been initiated.

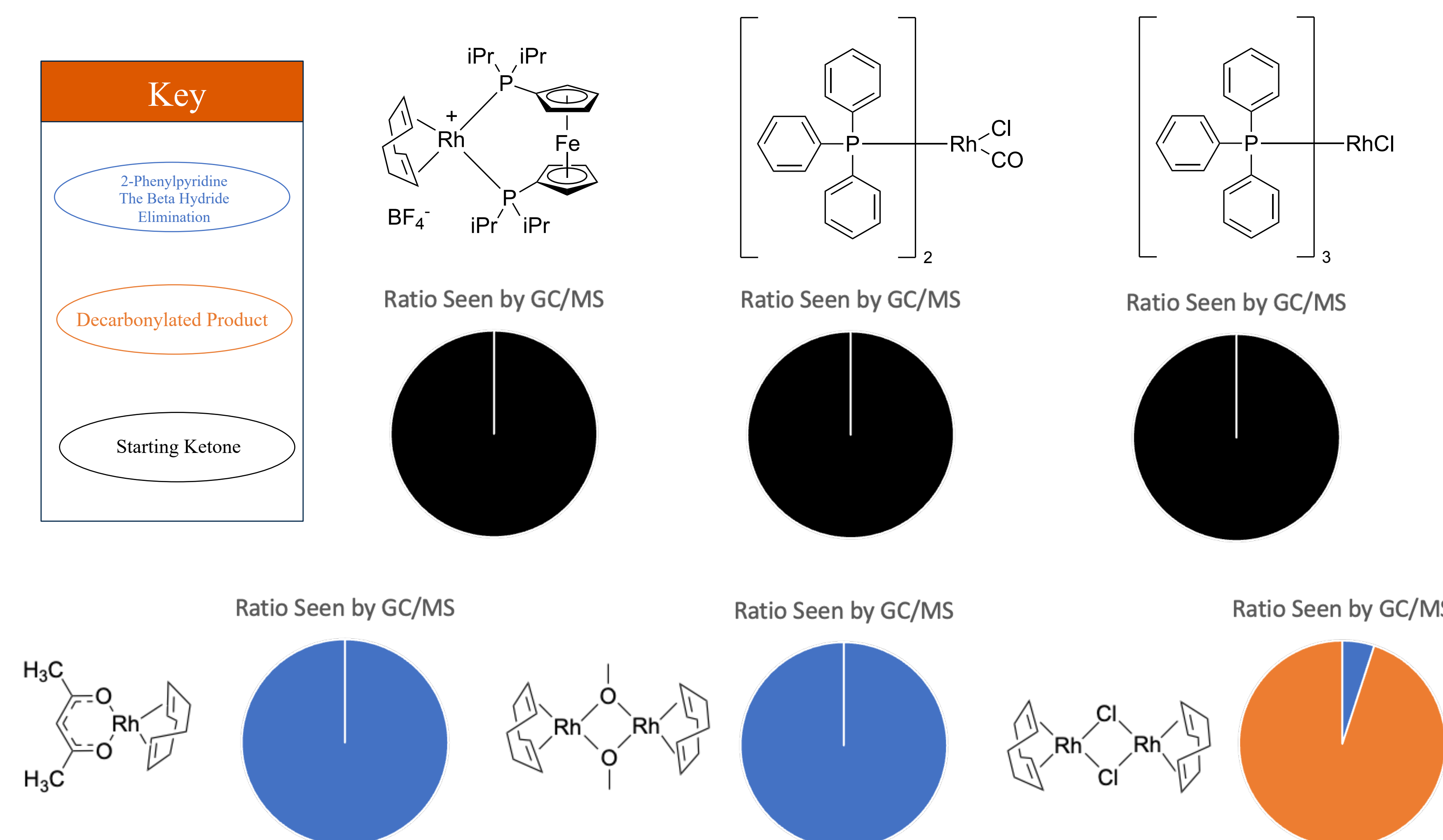
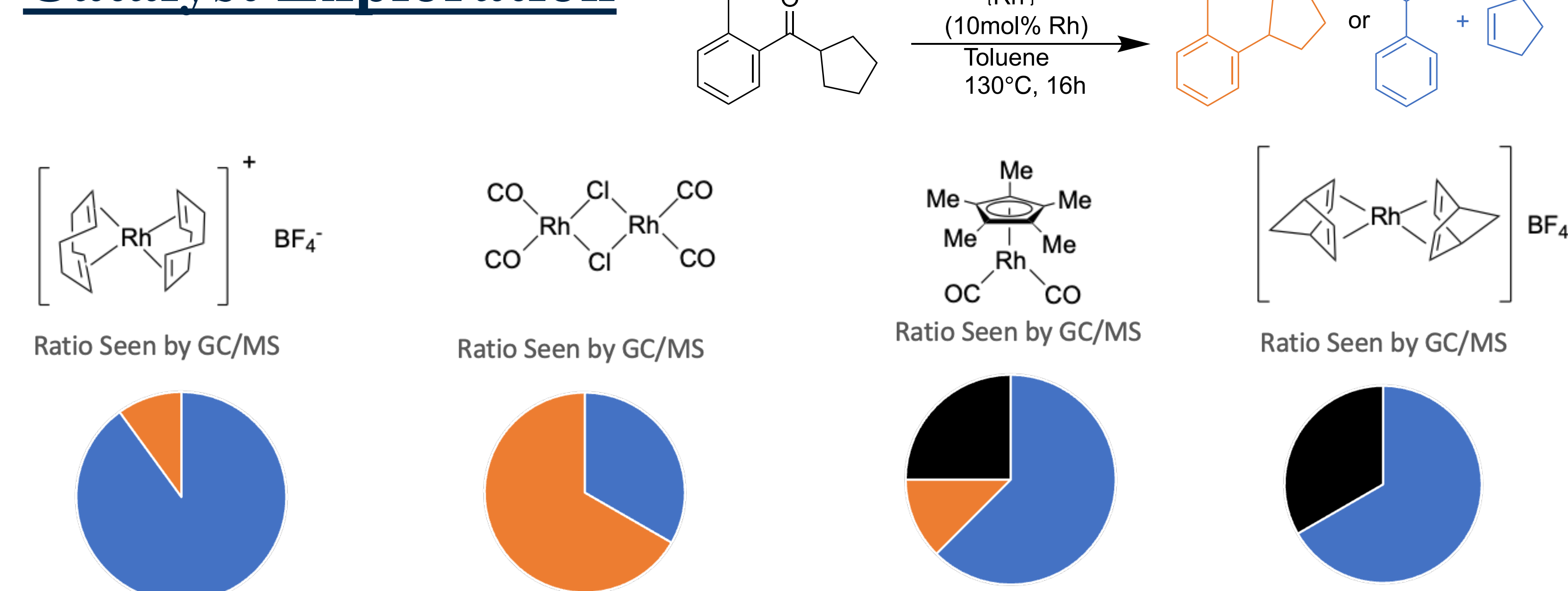
Mechanism of Decarbonylation



- This reaction can follow one of two pathways, either the **decarbonylation reaction** or the **beta hydride elimination**.

- When the beta hydride elimination occurs, 2-phenylpyridine is the only peak seen on the GC/MS. The alkene is volatile.

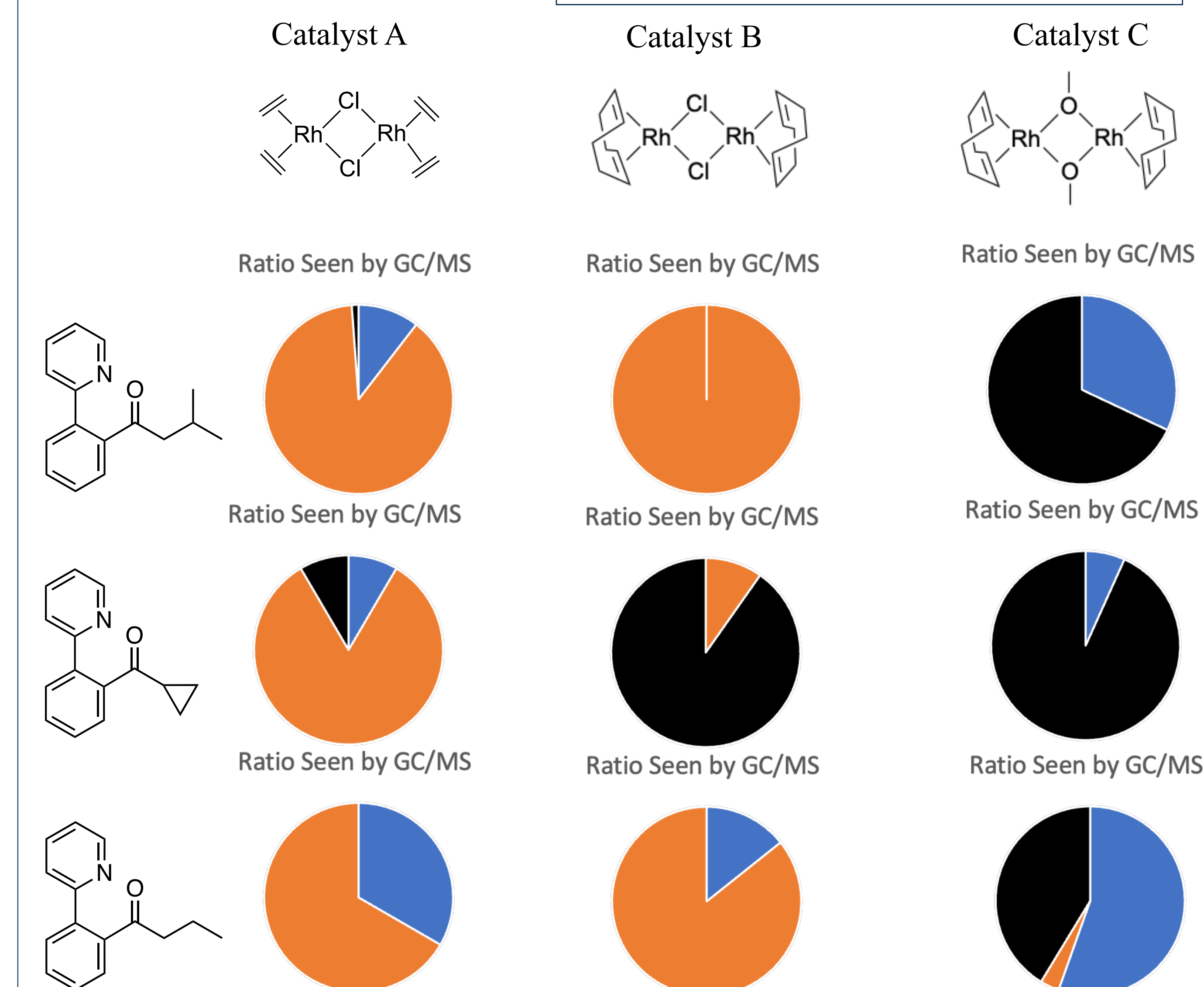
Catalyst Exploration



Selectivity of Other Ketones

Key:

2-Phenylpyridine ● Decarbonylated Product ● Starting Ketone ●



Future Work

- Optimize efficiency and selectivity
- Expand the library of ketones and decarbonylated products
- Synthesize and characterize the following decarbonylated products
- Examine the relative rates of the decarbonylation and elimination processes

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