4-12-2024

# The Breaking of Carbon-Carbon Bonds in Alkyl Ketones

Jenna R. Mustapha
*Hope College*

Jordan K. Montgomery
*Hope College*

Karen M. Nimtz
*Hope College*

Ainsley G. VandenBrink
*Hope College*

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

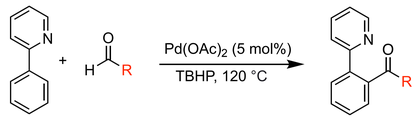
*Jenna R. Mustapha, Jordan K. Montgomery, Ainsley G. VandenBrink, Karen M. Nimtz, Jeffrey B. Johnson**
*Hope College, Holland, MI*

For more information, contact:
Jeffrey B. Johnson
Hope College
jjohnson@hope.edu

## 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.

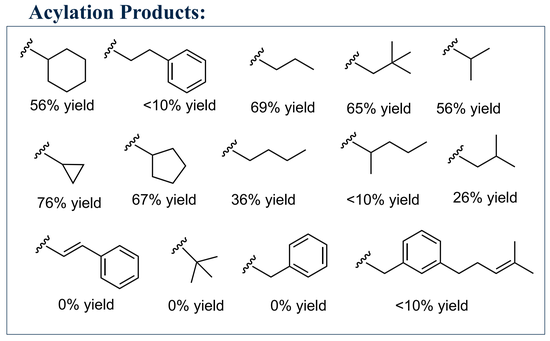
## Acylations for Ketone Formation




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

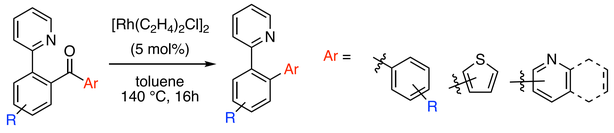
**Acylation Products:**

R =



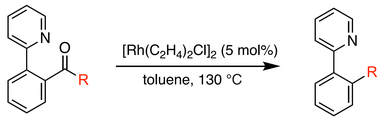

Baslé, B.; Shuai, L. *Adv. Synth. Catal.* **2010**, 352(7), 1145-1149.

## Decarbonylation



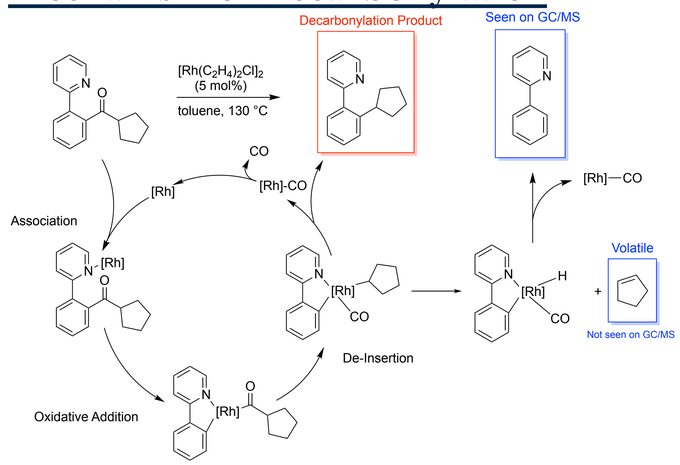

- 29 examples of different aryl groups were previously tested with the decarbonylation reactions with ~73-98% yield.

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.



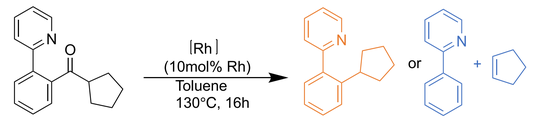

- Due to the high success rates of the aryl groups, exploration of alkyl groups has been initiated.

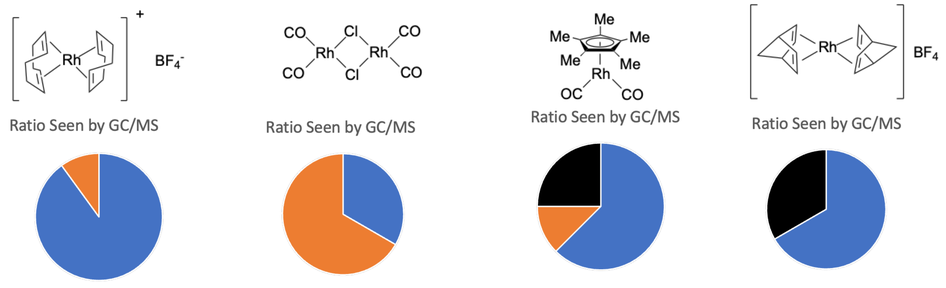
## Mechanism of Decarbonylation

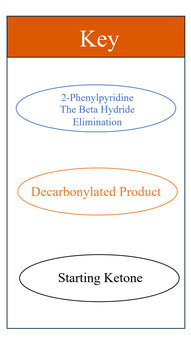


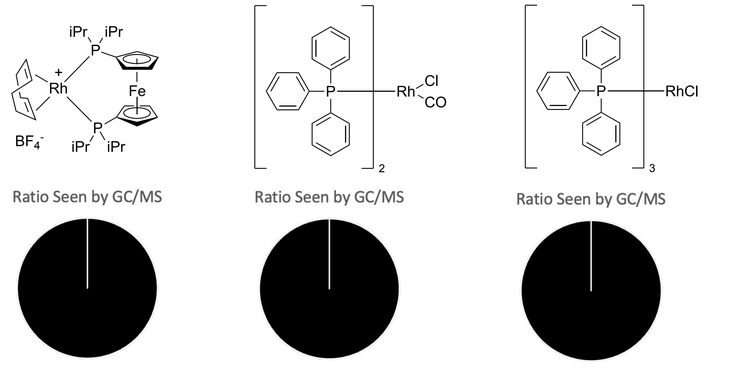

- This reaction can follow one of two pathways, either the decarbonylation reaction or the beta hydride elimination.
- When the beta hydride elimination occurs, 2-phenylpyridine is the only peak seen on the GC/MS. The alkene is volatile.

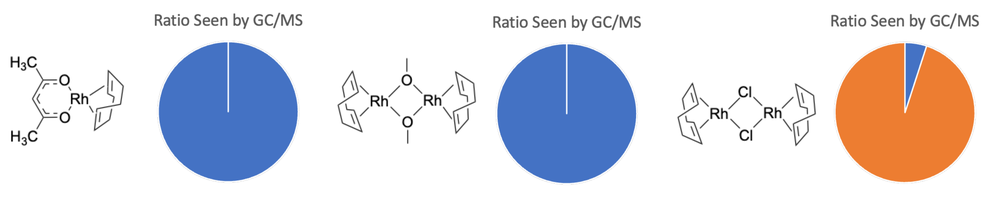
## Catalyst Exploration



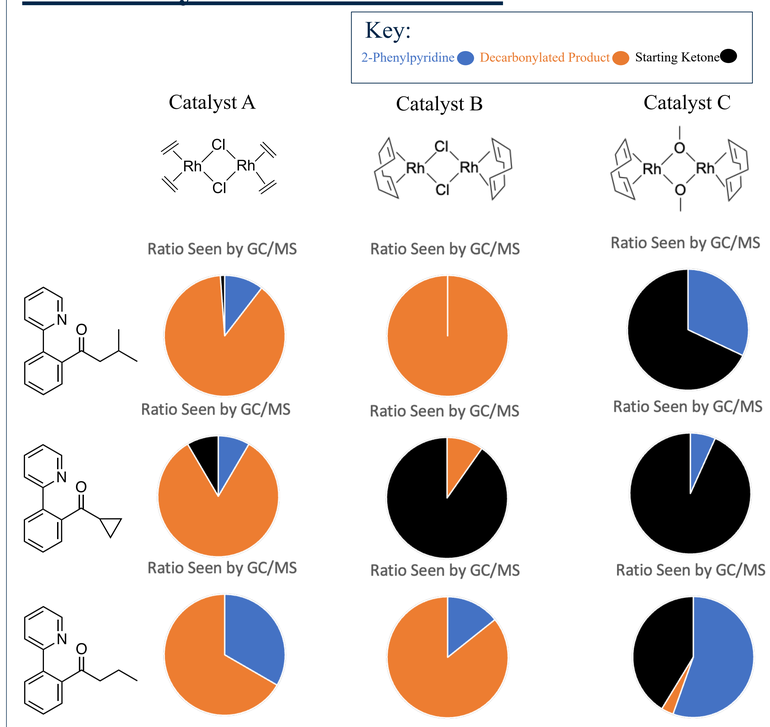




## Selectivity of Other Ketones




## Future Work

- Optimize efficiency and selectively
- 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

## Acknowledgements

- Johnson Lab Members, Past and Present
- Hope College Chemistry Department
- NSF: CHE-17116411
- Schaap Endowed Fund for Undergraduate Research
- Organic Synthesis Inc. Summer Research Grant