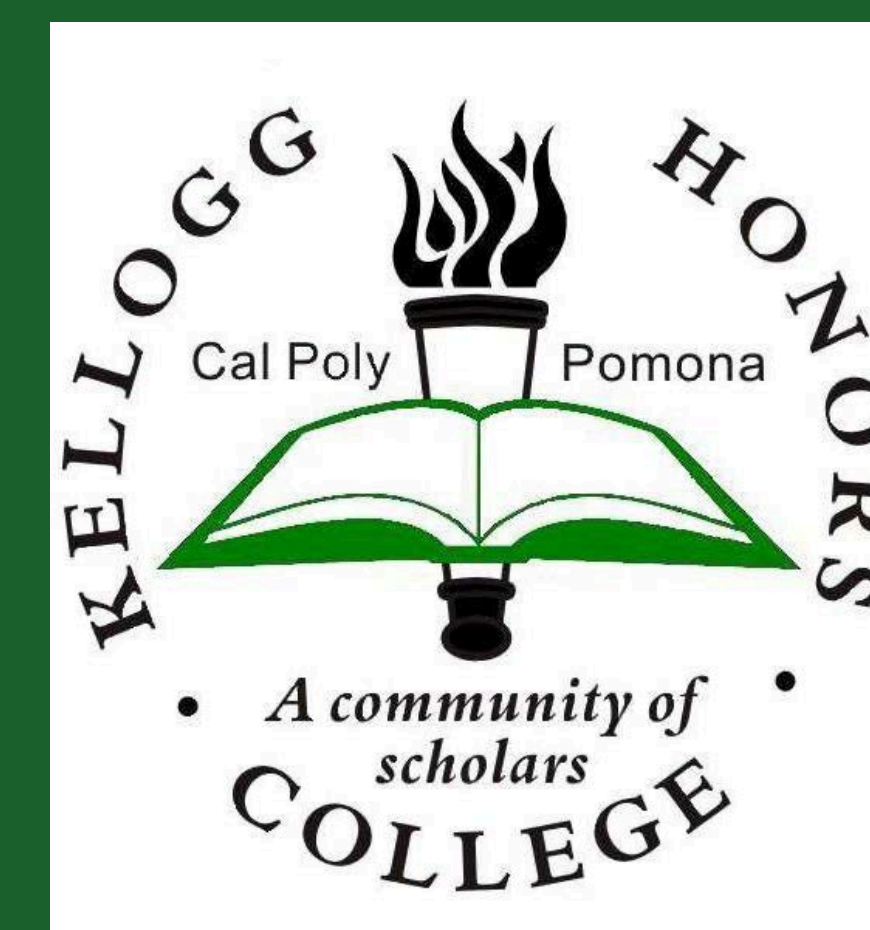




# Decarbonylation of Ketones with Bidentate N-Heterocyclic Carbene Nickel Complexes

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Kellogg Honors College Capstone Project



## What is decarbonylation?

- Removing CO (carbonyl) from a molecule
- Significant for pharmaceutical and fine chemical production
- Alternative route for synthesizing carbon-carbon bonds
- Difficult to achieve
- First decarbonylation of ketones with nickel recently reported

## Goals

- Synthesize new nickel catalysts
- Test nickel catalysts in decarbonylation
- Determine effect of ligand sterics in *decarbonylation*

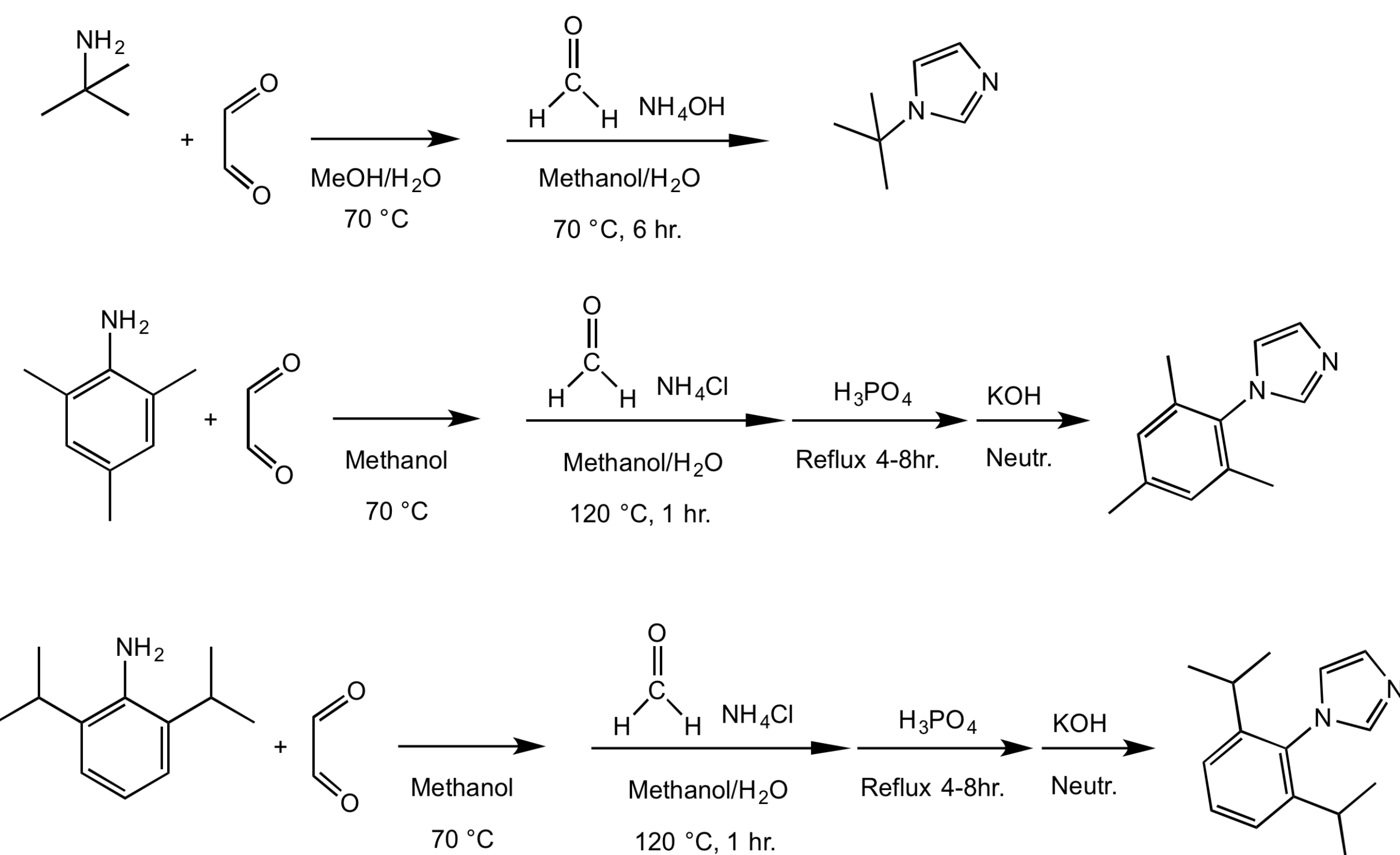


Inert Atmosphere Glovebox

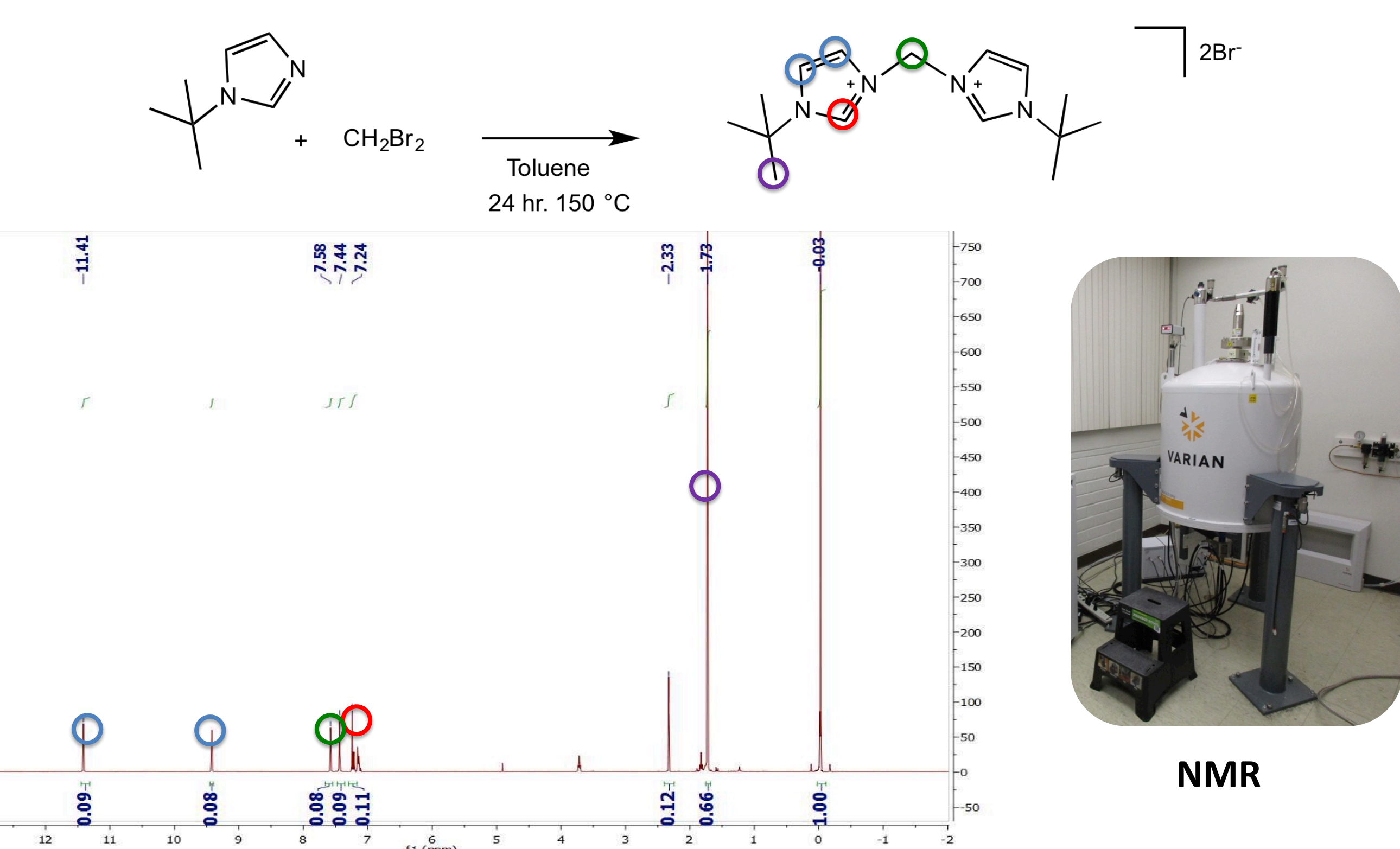
Schlenk/Vacuum Lines

Solvent Purification System

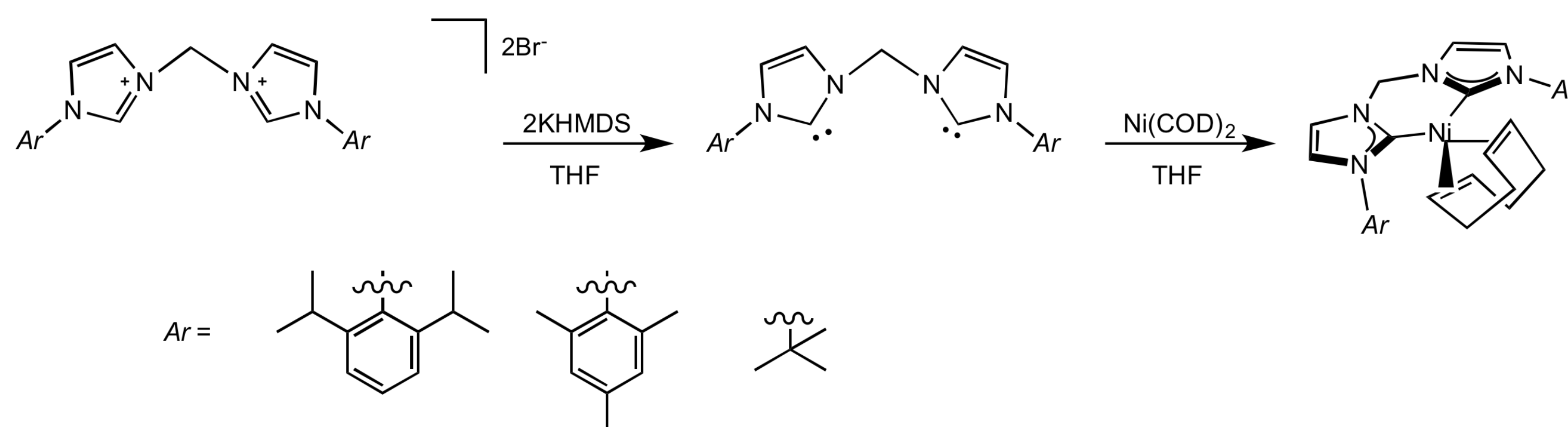
## Preparation of ligand precursors



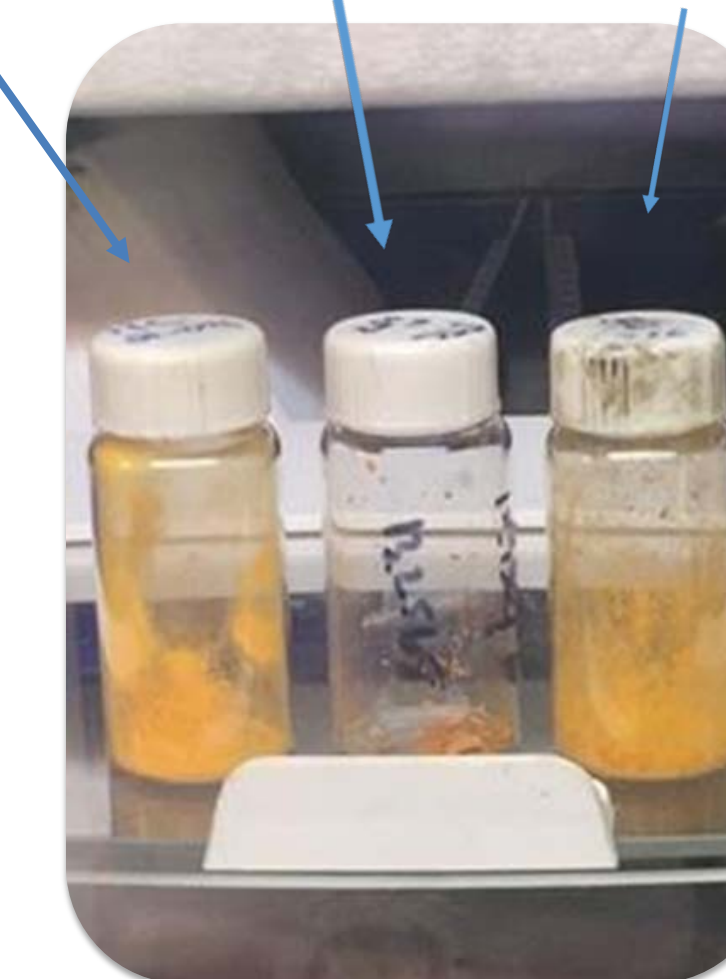
## Ligand Synthesis (bismidazolium salt)



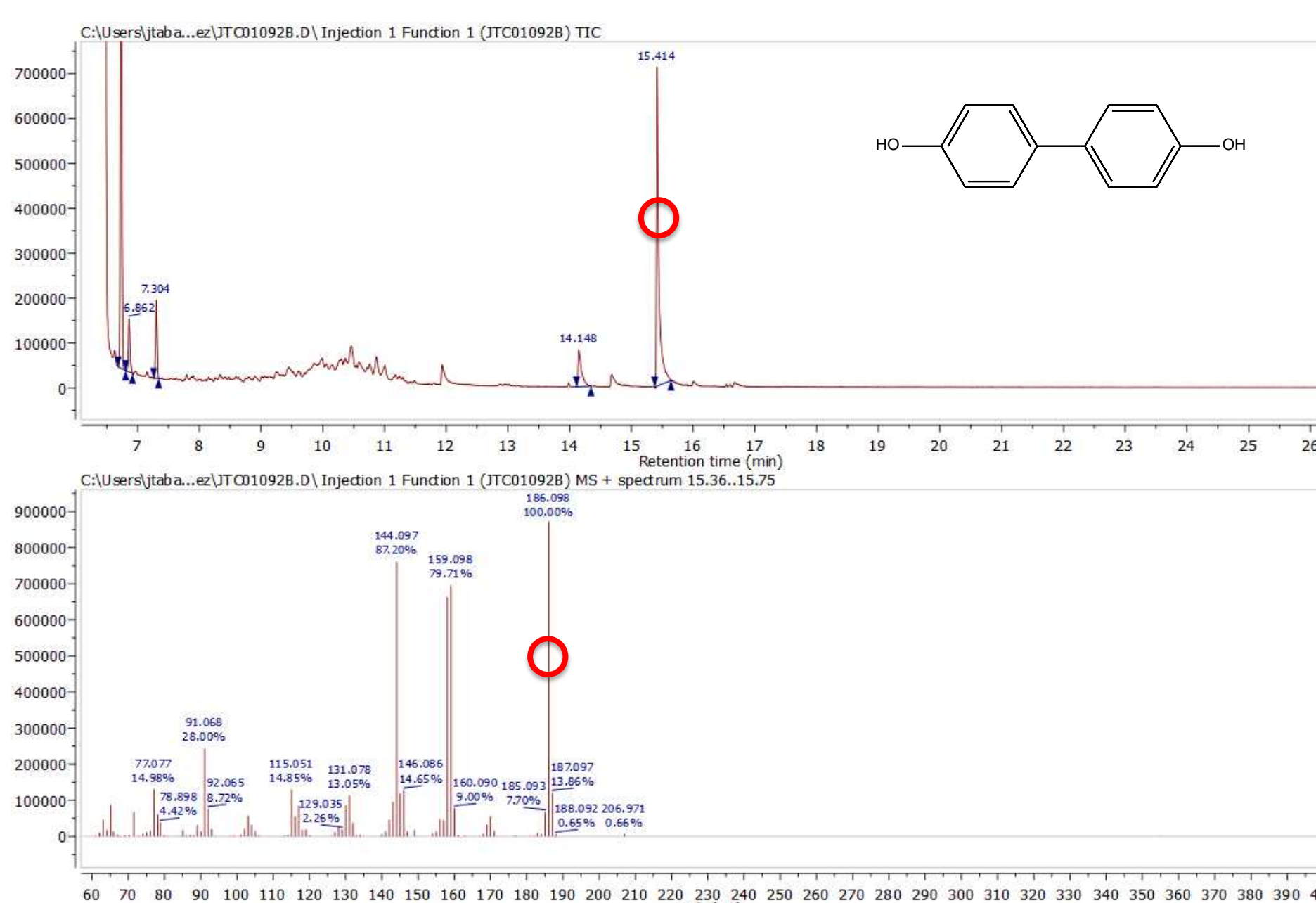
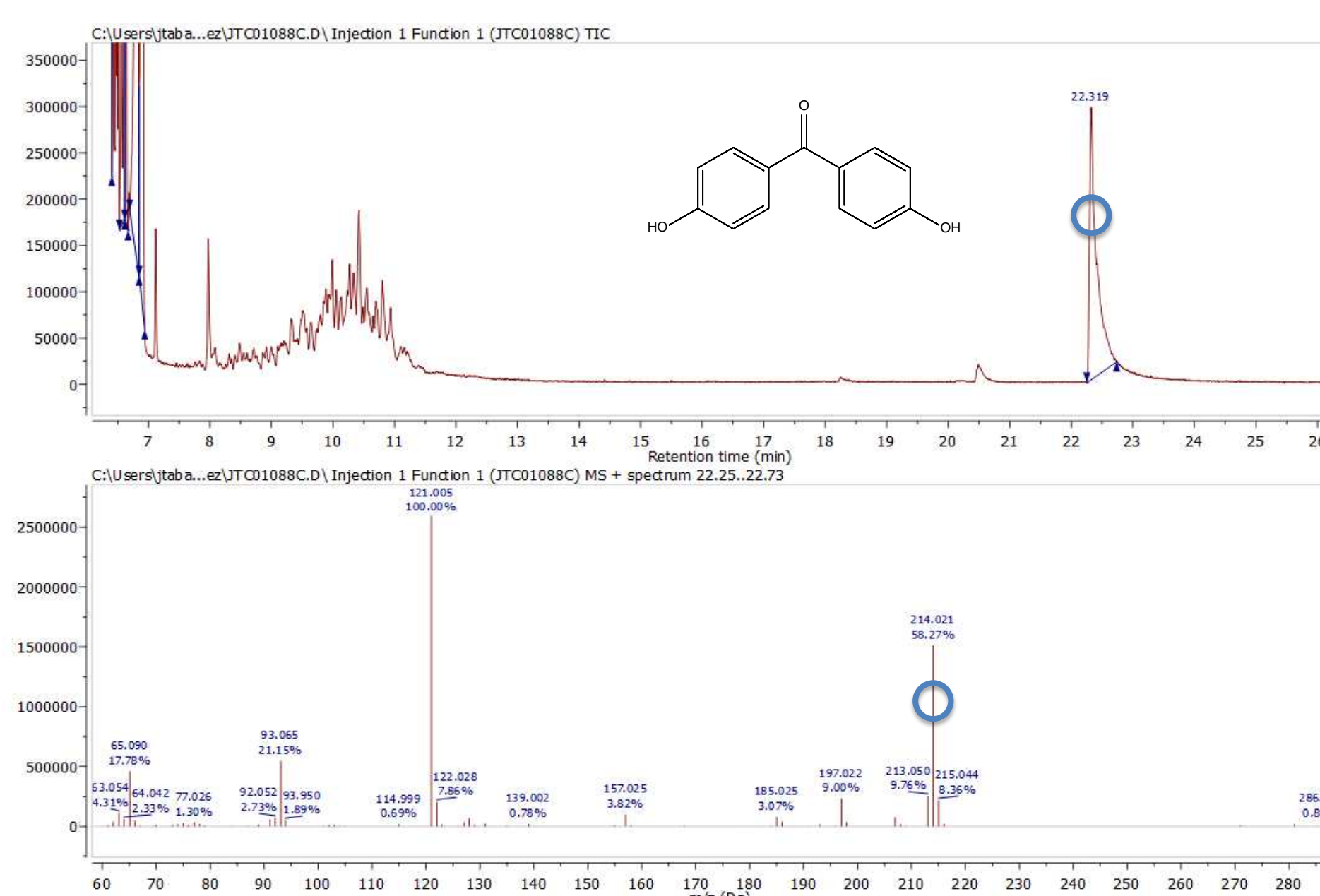
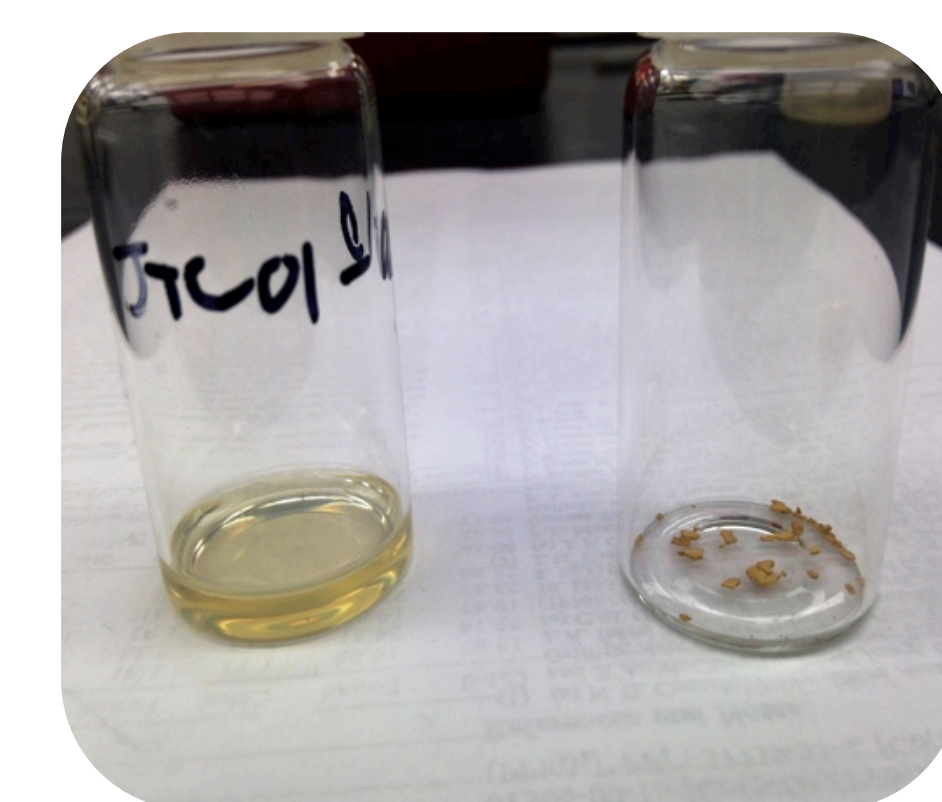
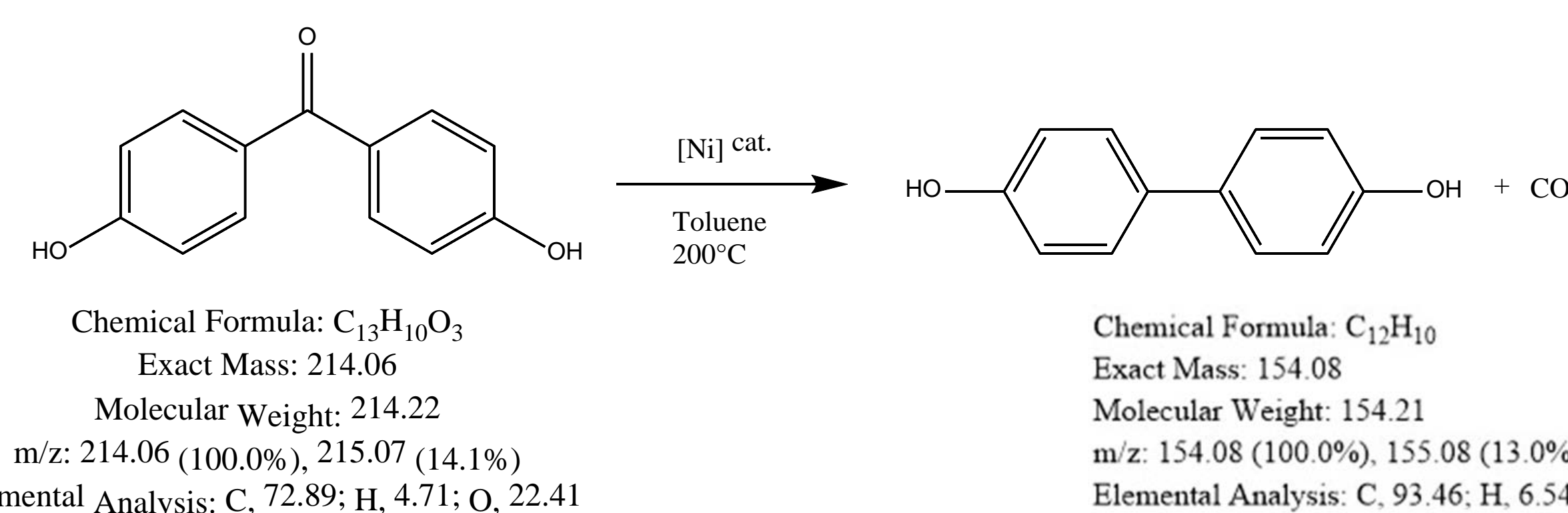
## Synthesis of nickel catalyst



tert-butyl complex mesityl complex dipp complex



## Decarbonylation of ketones

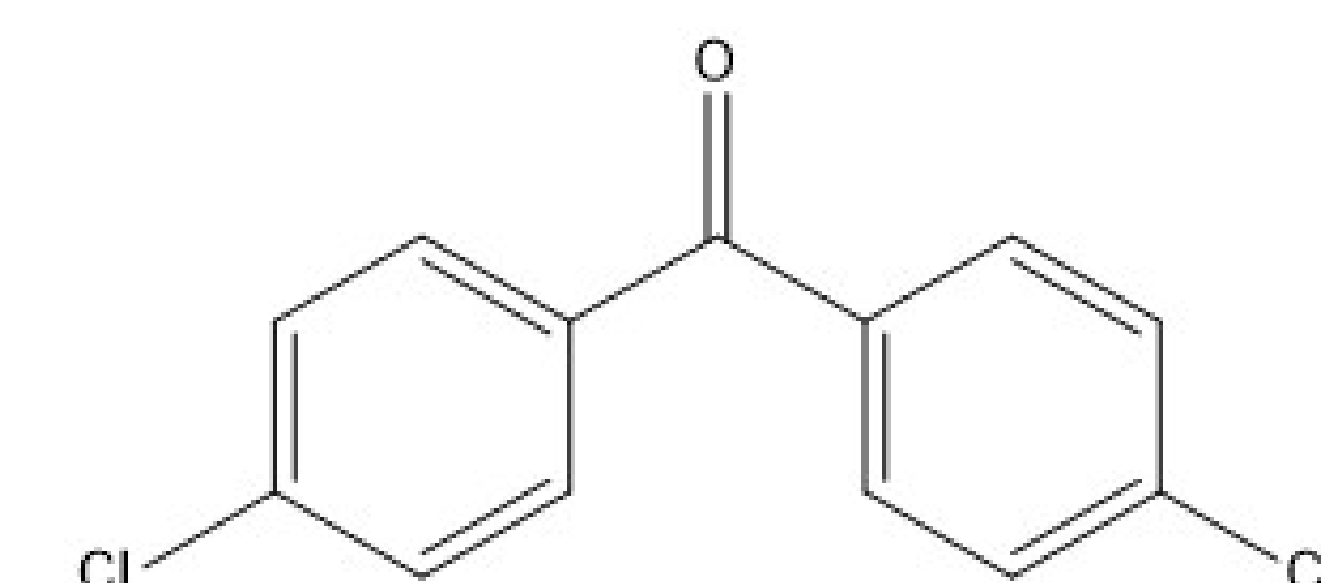


## Decarbonylation Reactions with other Ketones

R group	[Ni] catalyst	Product identified?
-H	<i>t</i> -butyl	Yes
-H	Mes	No
-NCCEt <sub>2</sub>	<i>t</i> -butyl	No
-NEt <sub>2</sub>	Mes	Yes
-OCH <sub>3</sub>	<i>t</i> -butyl	No
-OCH <sub>3</sub>	Mes	No
-OH	<i>t</i> -butyl	No
-OH	Mes	Yes
-CH <sub>3</sub>	<i>t</i> -butyl	Yes
-CH <sub>3</sub>	Mes	Yes

## Conclusions and Directions

- Initial decarbonylation reactions demonstrated
- Utilize preliminary data to improve conversion
- Expand scope to additional functionalized ketones
- Develop new nickel catalysts



Special thanks to LSAMP, the Goldstein Family, the Cal Poly Pomona College of Science, Department of Chemistry, and RSCA.

## References

- Brendel, M. et al. *Angew. Chemie- Int. Ed.* **2014**, 53, 8741-8745.  
Cowie, M. et al. *Organometallics*, **2008**, 27, 692.  
Liu, J. et al. *Synthesis (Stuttg.)*. **2003**, 17, 2661.  
Morioka, T. et al. *J. Am. Chem. Soc.* **2017**, 139, 1416-1419.  
Smith, J. M. et al. *Inorg. Chem.* **2006**, 45, 9771.

