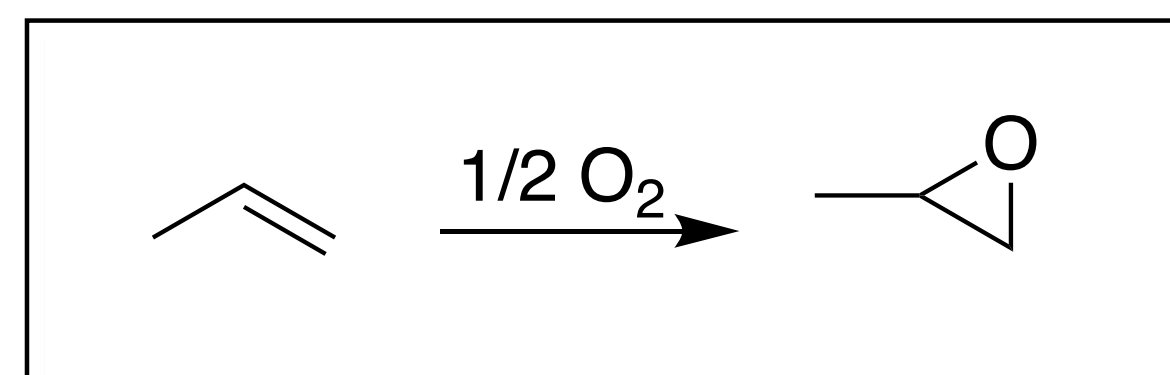
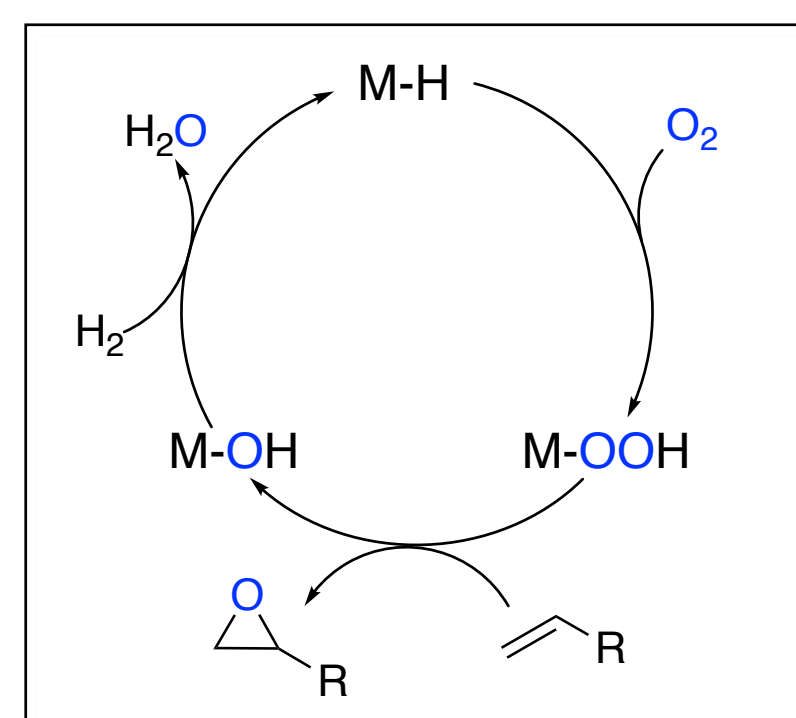


Introduction and Research Goals

- The production of propylene oxide occurs on a scale of 6 million tons per year¹. Currently, the main production of propylene oxide uses chlorine, which is environmentally detrimental. Alternative options that are more environmentally friendly are cost prohibitive. Ideally, oxygen could be used as a chemical oxidant, as it is cheap, easy to work with, and environmentally benign.

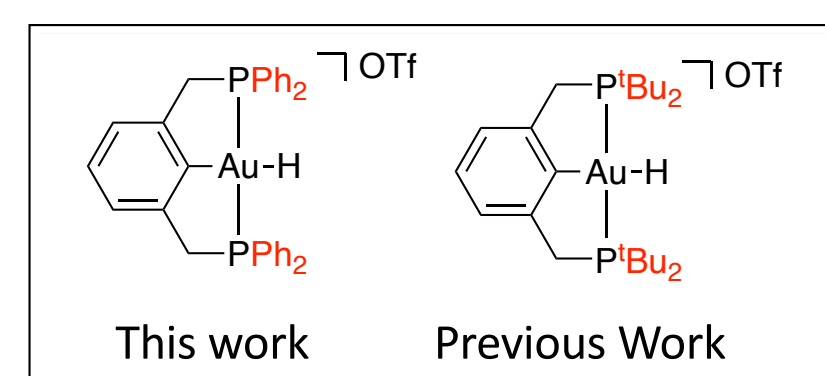
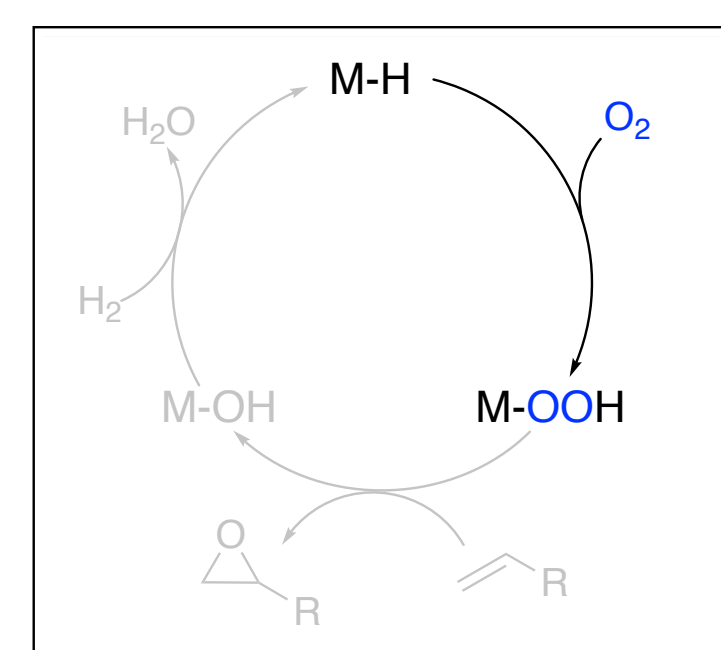
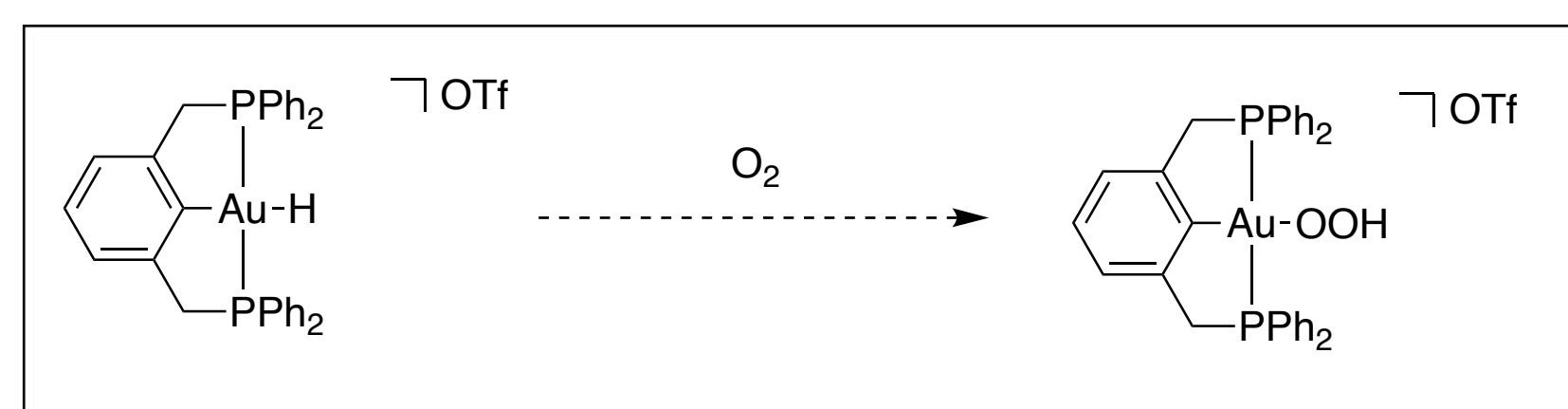


- The Goldberg Group's approach to sustainable oxidations is through a three-step catalytic cycle. The cycle starts with an O₂ insertion, followed by an oxygen atom transfer, and finally hydrogenolysis.



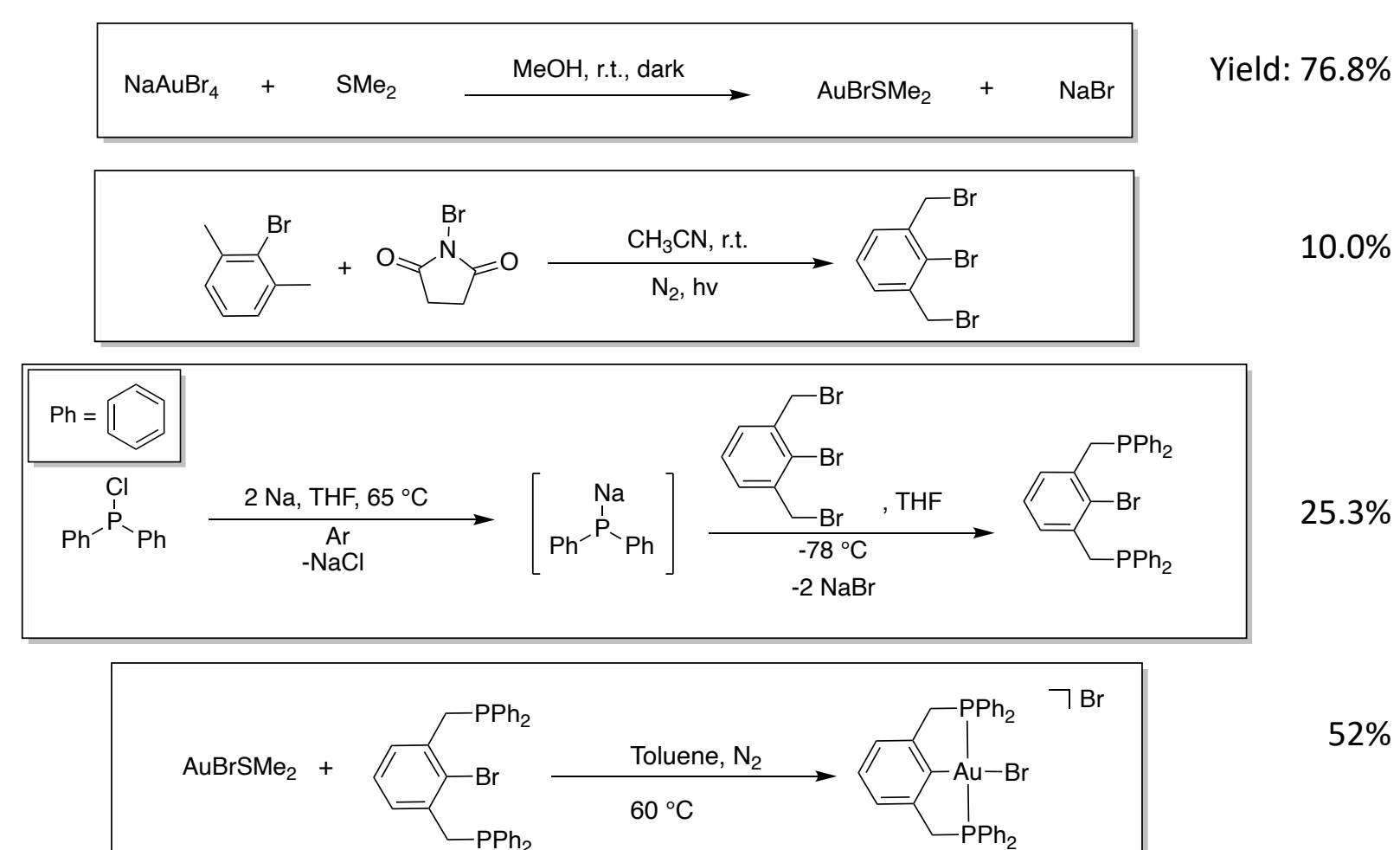
Project Goals

- The primary goal of this project was to focus on the O₂ insertion step with a gold pincer complex. Previous group work with Au(III) complexes⁶ have shown the viability of the catalytic cycle.

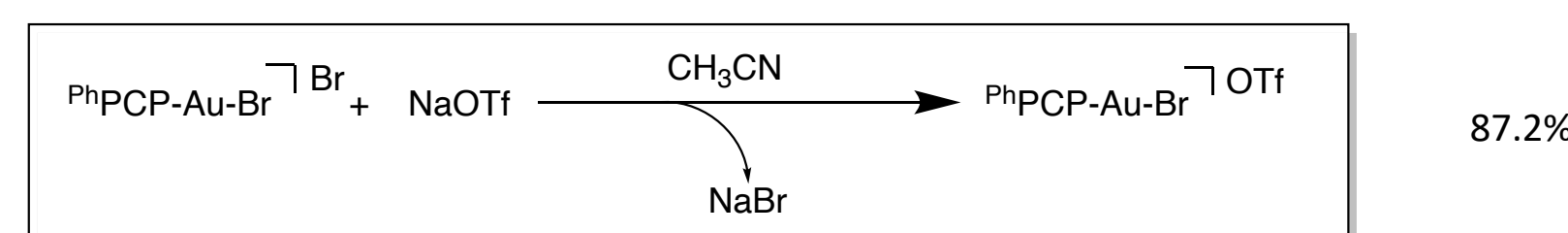


Synthesis of Gold (III) Pincer Complex

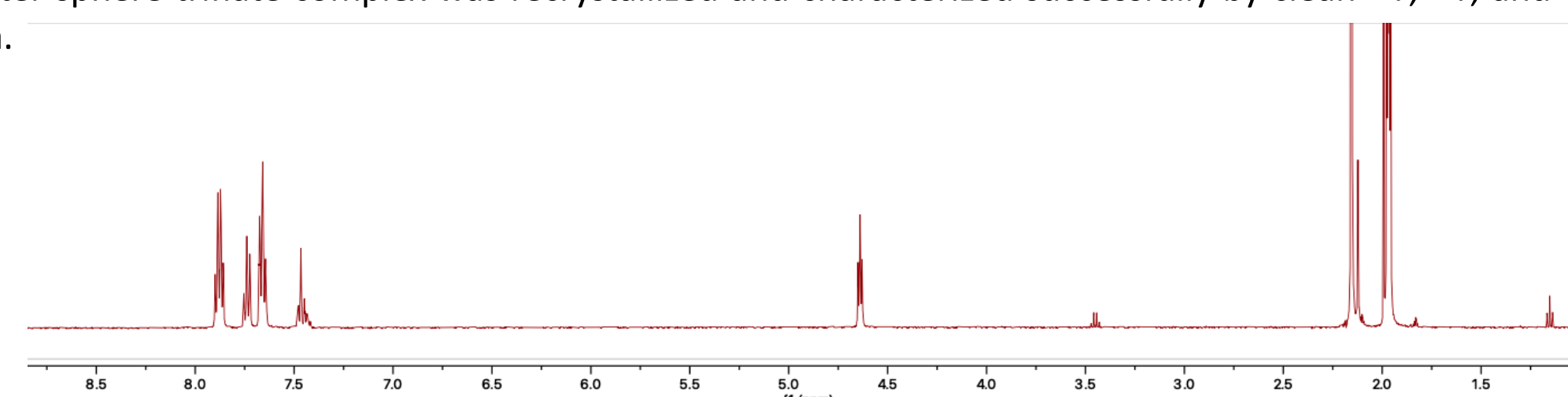
- The synthesis of the gold (III) pincer complex followed literature procedures^{2, 3, 4, 5, 6}



Novel Outer Sphere Triflate



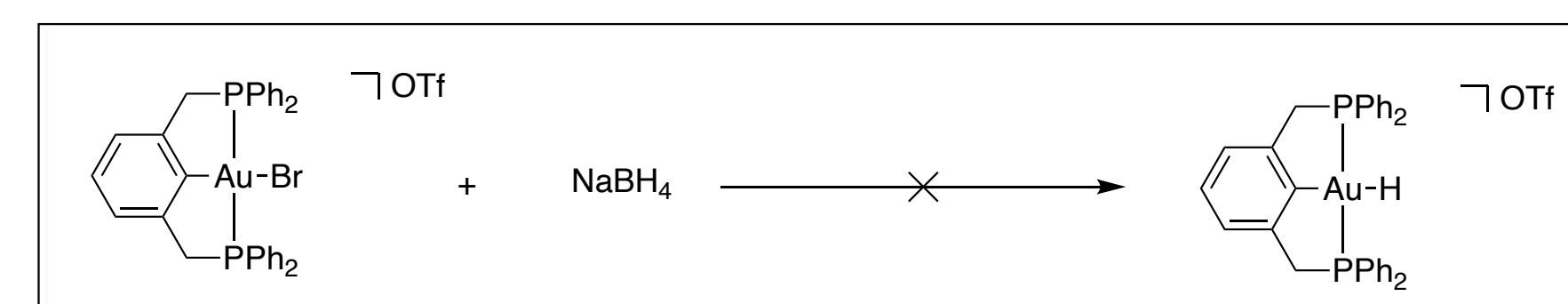
- The outer sphere triflate complex was recrystallized and characterized successfully by clean ³¹P, ¹⁹F, and ¹H NMR spectra.



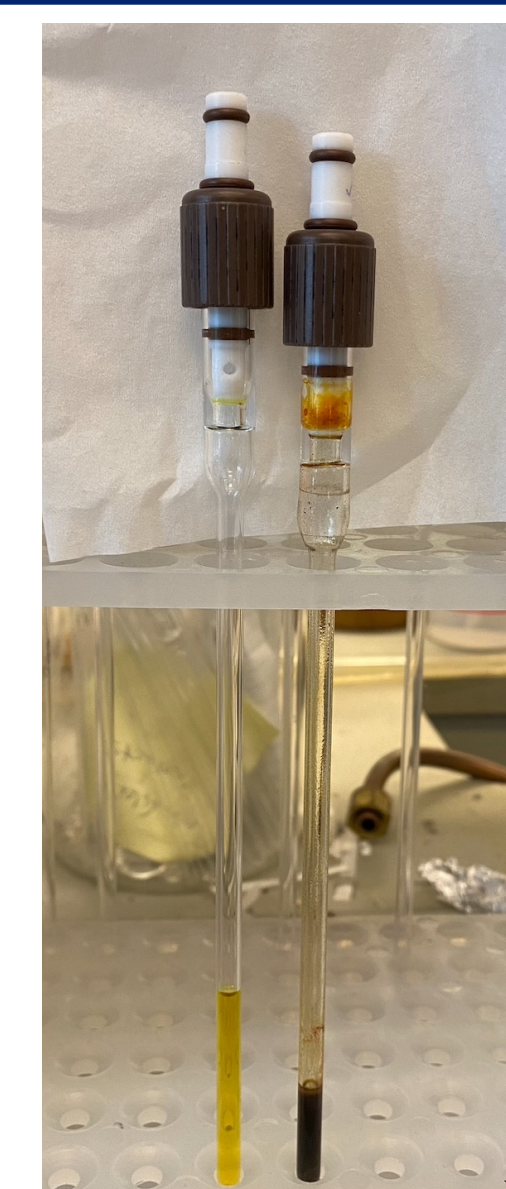
- ¹H NMR (500 MHz, CD₃CN)
- The peaks correlate to the desired product, with minimal solvent contamination.

Attempted Synthesis of Gold Hydride

- The attempted synthesis of the gold hydride led to unexpected and unidentifiable reactivity. The reaction was attempted in acetonitrile in air, air free, and on an NMR scale. The reaction was also attempted in methanol on an NMR scale.

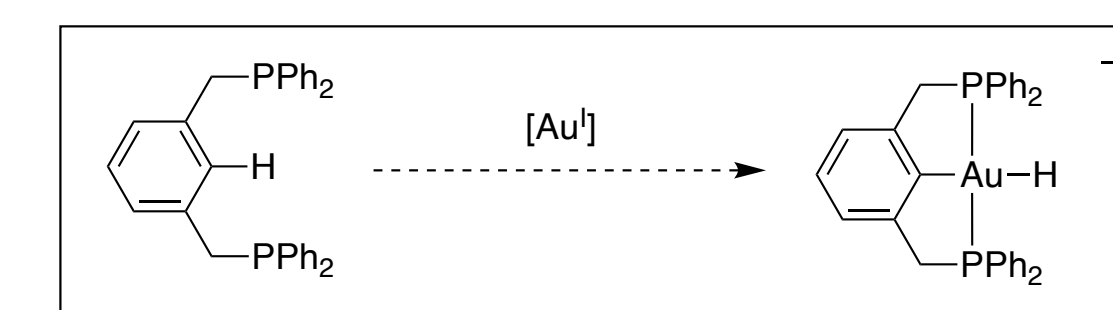


- Further analysis revealed that the solvent was interacting directly with the gold bromide complex. The complex reacted with MeOH, but not CH₃CN or CDCl₃.
- The reaction between the Au-Br complex and NaBH₄ led to unidentifiable nonproductive reactivity. Solid precipitated out, and ³¹P NMR showed an intractable mixture of products, consistent with decomposition. Possible explanations could be:
 - The NaBH₄ reduces the ligand instead of the Br
 - The hydride was created, but is too unstable

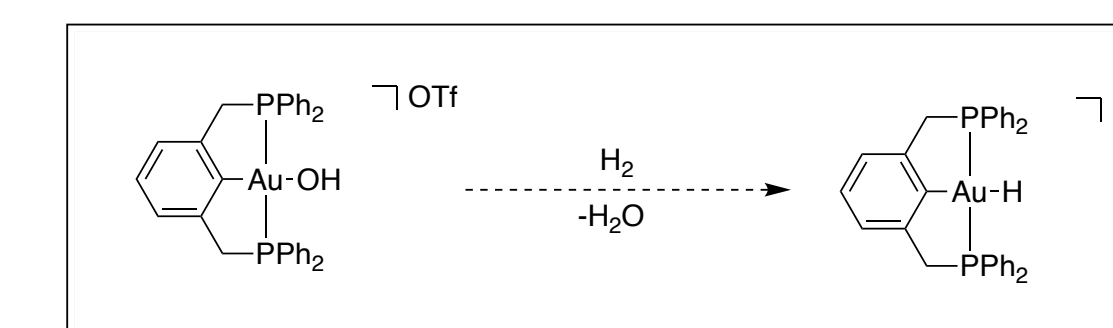


Future Work

- The formation of the hydride is still a goal, but alternative reactions might be necessary to create the hydride. Some possibilities include:
- Direct formation of Au-H by C-H oxidative addition



- Using an alternate hydride source, such as LiHBET₃ or NaBH₃CN
- Another avenue of future research is to try to synthesize the gold hydride via a hydrogenolysis reaction of the gold hydroxide. This has been successful for analogous Au complexes.



Conclusions

- The reactivity of the diphenyl gold pincer complex was surprisingly different from that of the di-tert-butyl complex.
- It is unclear if the sterics and electronics of the two ligand systems are promoting different reactions.
- The diphenyl ligand and diphenyl gold bromide complex were made and characterized, with attempted reactions under different conditions to see if the hydride could be synthesized

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