Rethinking CO2 Reducing Heterogeneous Catalyst Precursors

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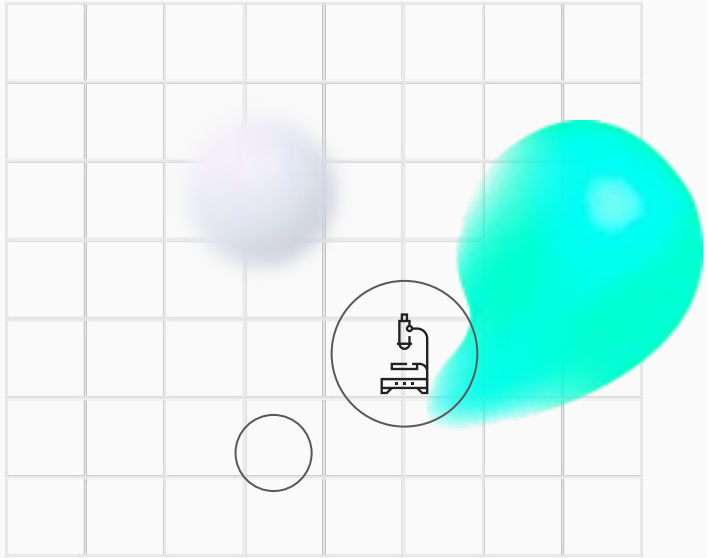
Introduction

- Catalyst Development has faced several challenges in recent years
  - Energy efficiency
  - Product selectivity
  - Scalability
- Challenges hinder the development of CO2 reduction becoming widespread method to deal with the pollutant
- Some of the most promising catalysts are heterogeneous catalysts; however:
  - Mechanisms are only briefly explored
  - Not fully understood in the context of CO_2 reduction

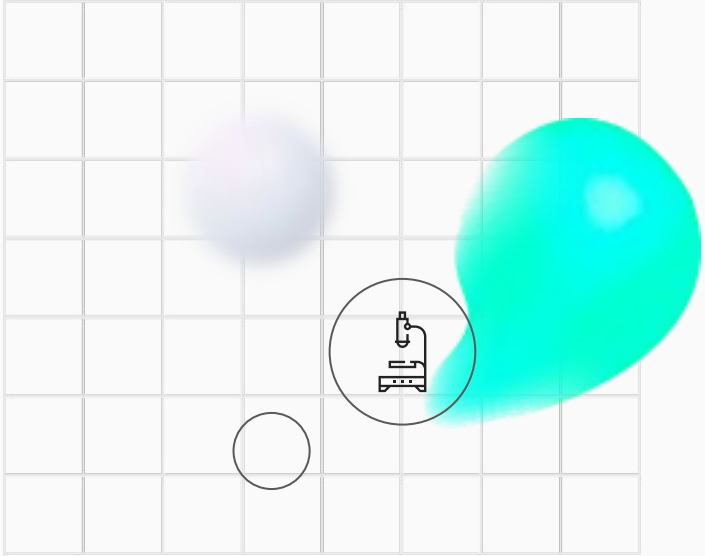


Objective

- Using previous studies, goal is to design molecular copper catalyst precursors
  - Will deposit atoms on catalyst surface
  - Aim to influence selectivity for carbon-carbon bond-forming reactions

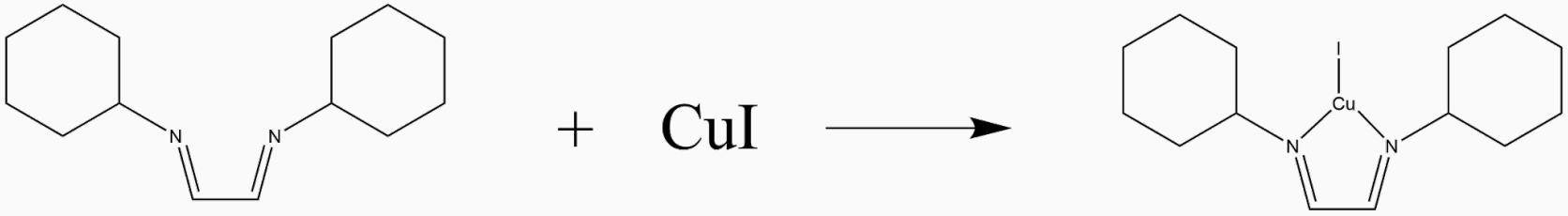
Ultimately:

How can ligand design be used to produce reliable precursors to solid copper catalysts with high activity and selectivity for the reduction of CO_2 to hydrocarbons?



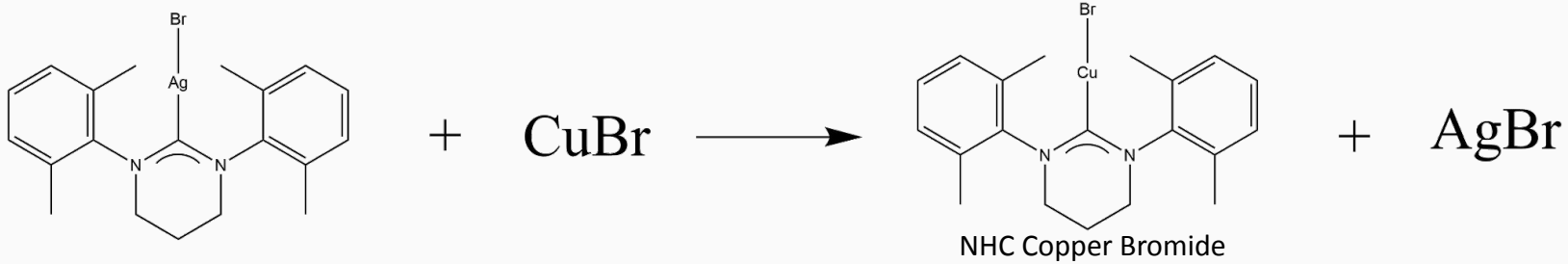
Reactions Developed:

Diimine Complex Rxn:



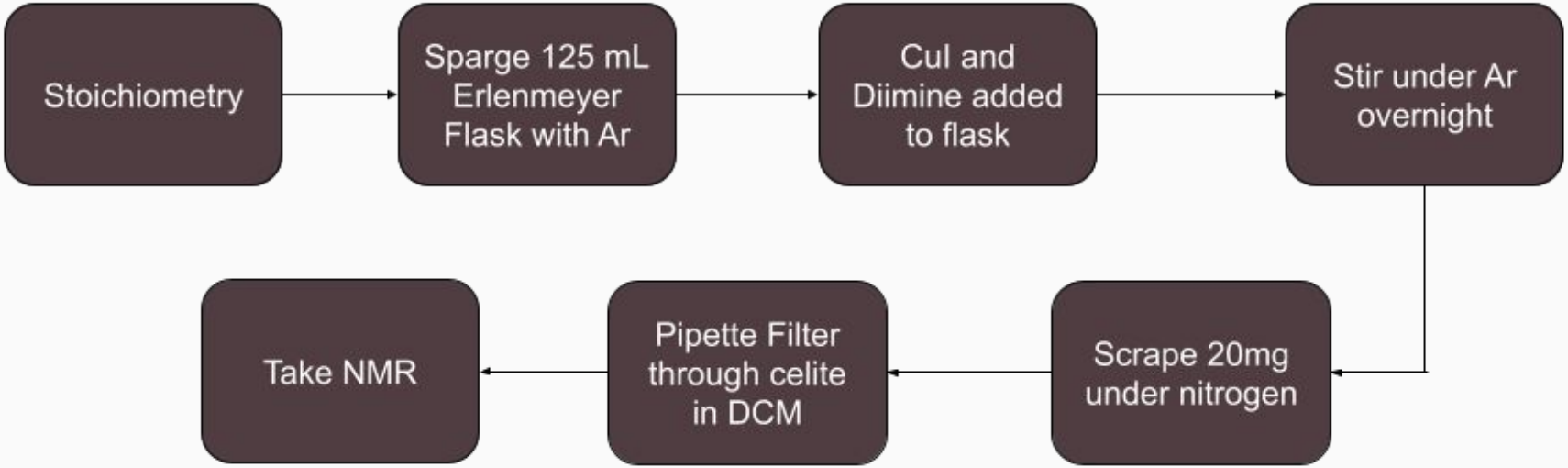
Diimine Copper Iodide

Diimine Complex Rxn:

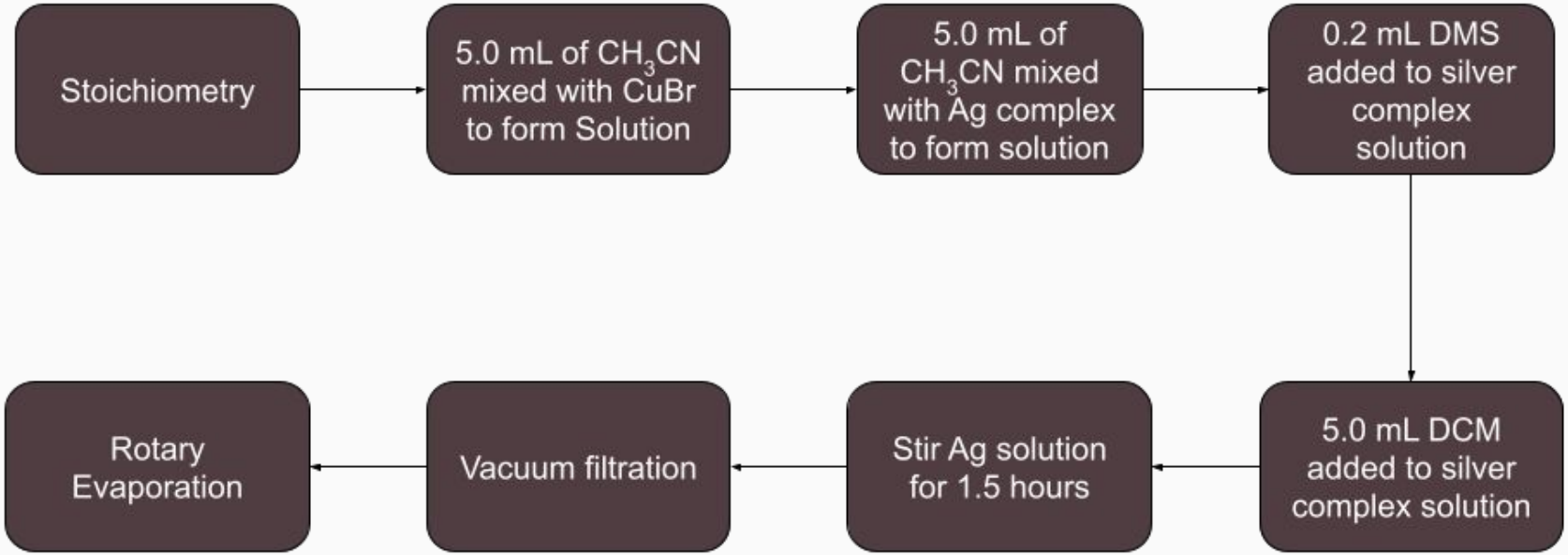


NHC Copper Bromide

Procedures – Diimine Complex

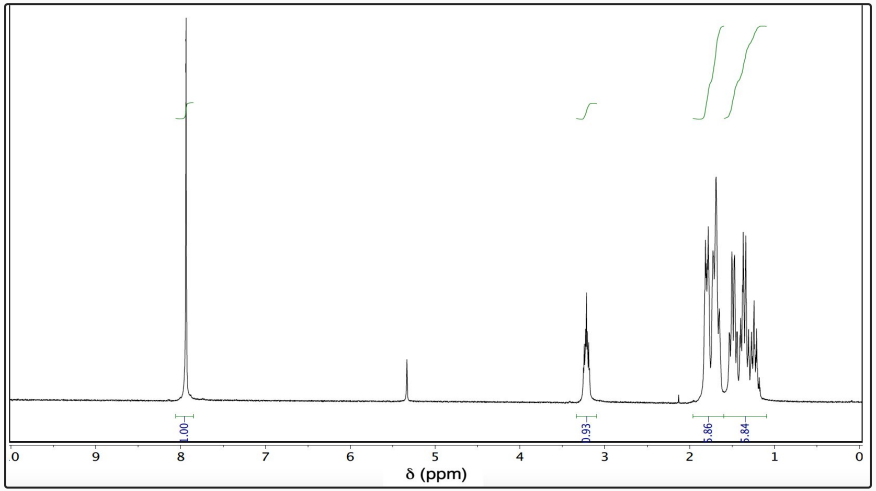


Procedures – Diimine Complex



Interpretations and Observations

- Diimine:
  - The spectra indicates that the reaction did yield a product for the diimine, as one would expect due a shift in shielding
  - The lack of solubility in DMSO and limited solubility in acetone indicate successful reaction
- Silver Complex
  - Immediately after CuBr solution was added to the silver complex solution, a tan color appeared.
    - Tan precipitate likely indicates silver bromide precipitation



Conclusions and Future Implications

- **Success of both molecules allows for CO2 to be used as hydrogen storage medium**
- Benchtop chemistry used to synthesize molecules
  - **Scalable reaction path created**
- Diimine copper iodide should bind easily to carbon monoxide because of two nitrogen donors
  - Promising to work with carbon-dioxide reducing catalysts
- NHC copper bromide does not simply produce AgBr precipitate
  - Carbene transferred to other metal, creating new carbene

References

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