



Optimizing Dioxomolybdenum Catalysts for the Conversion of Biomass to Chemicals

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Introduction

- Petroleum is currently the source of olefins
- Problem: Fossil fuel resources are the number one cause of pollution and petroleum products are non-renewable
- Solution: Switch to sustainable resources, for example biomass derived resources, that may supplement and replace fossil resources

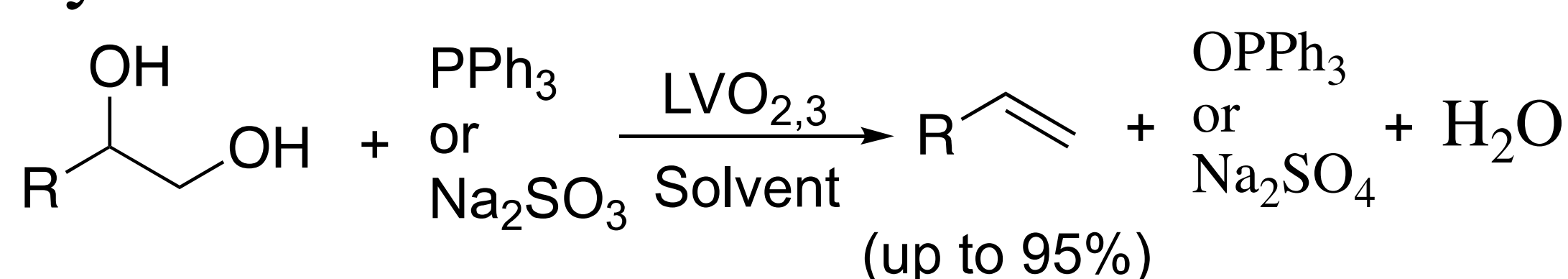


Deoxydehydration (DODH)

- Single step process
 - This reaction converts biomass derived vicinal diols into olefins by employing a metal catalyst and a variety of reductants
- $$\text{R-CH(OH)-CH(OH)-R} + \text{Red} \xrightarrow[\text{Solvent}]{\text{LMoO}_2} \text{R-CH=CH-R} + \text{ORed} + \text{H}_2\text{O}$$

Vanadium-Catalyzed DODH

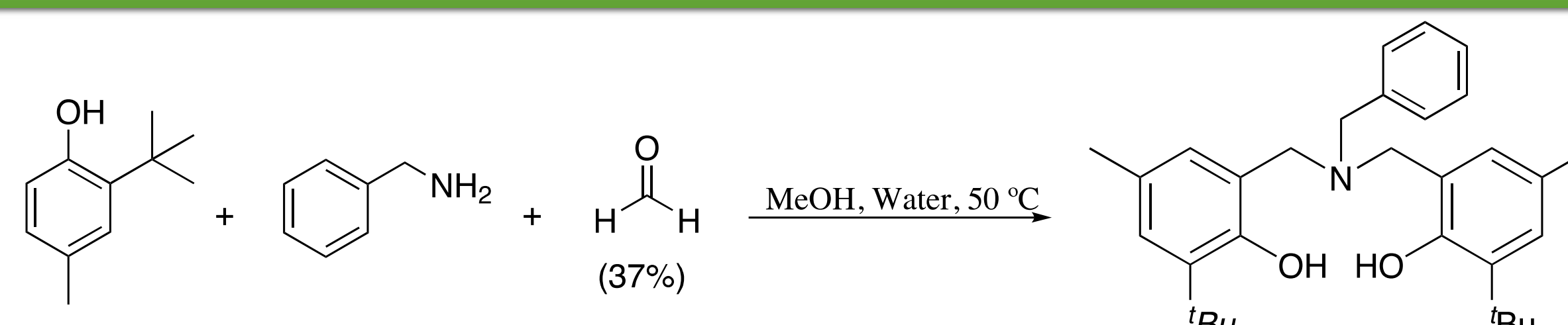
Advances in the Vanadium employed DODH were made in the Nicholas group. Dr. Nicholas and his team employed a variety of Vanadium catalysts with varying ligand groups and found to have excellent results in terms of conversion rates and yields



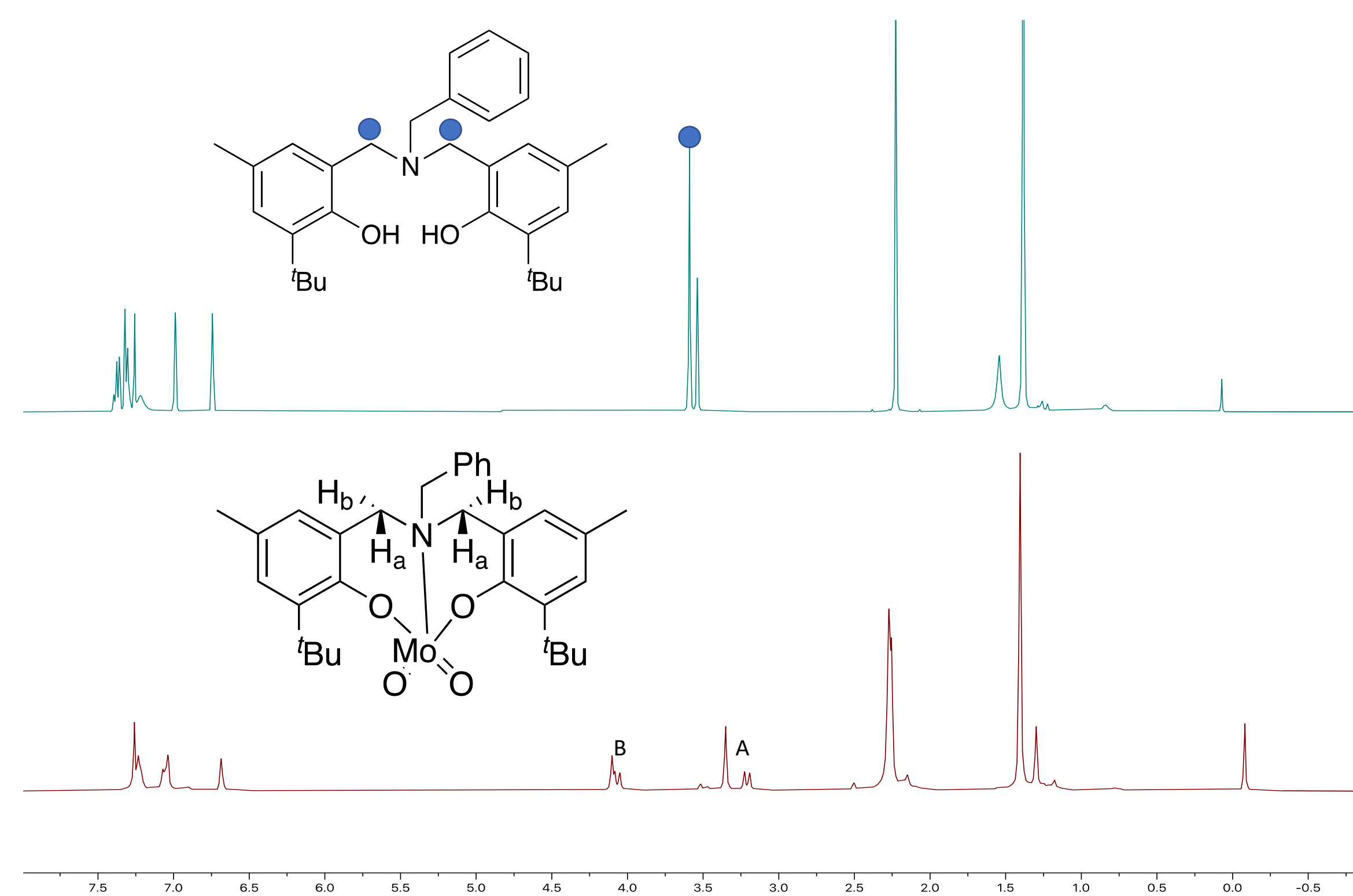
Strategy

- Synthesize and explore the reactivity of molybdenum catalysts, to catalyze a DODH reaction.
- Change solvents and temperatures to understand optimal DODH conditions

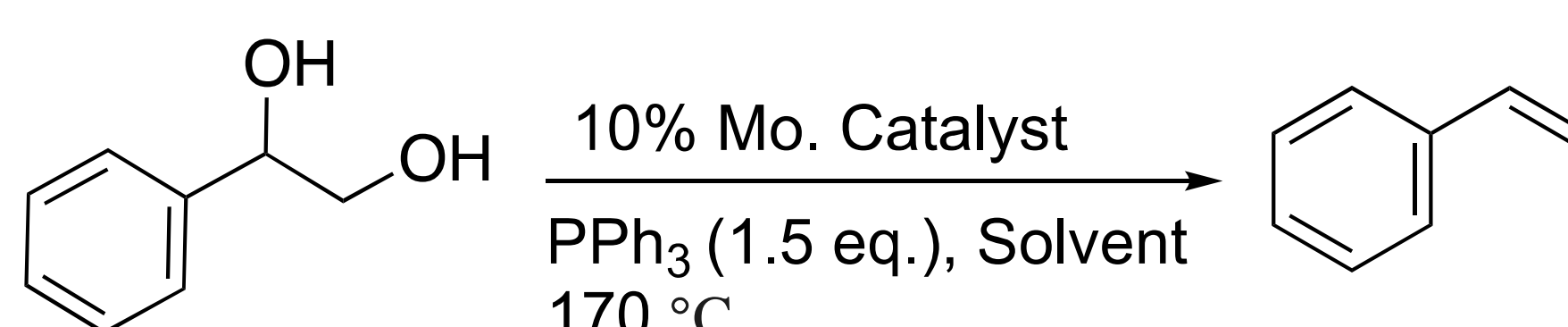
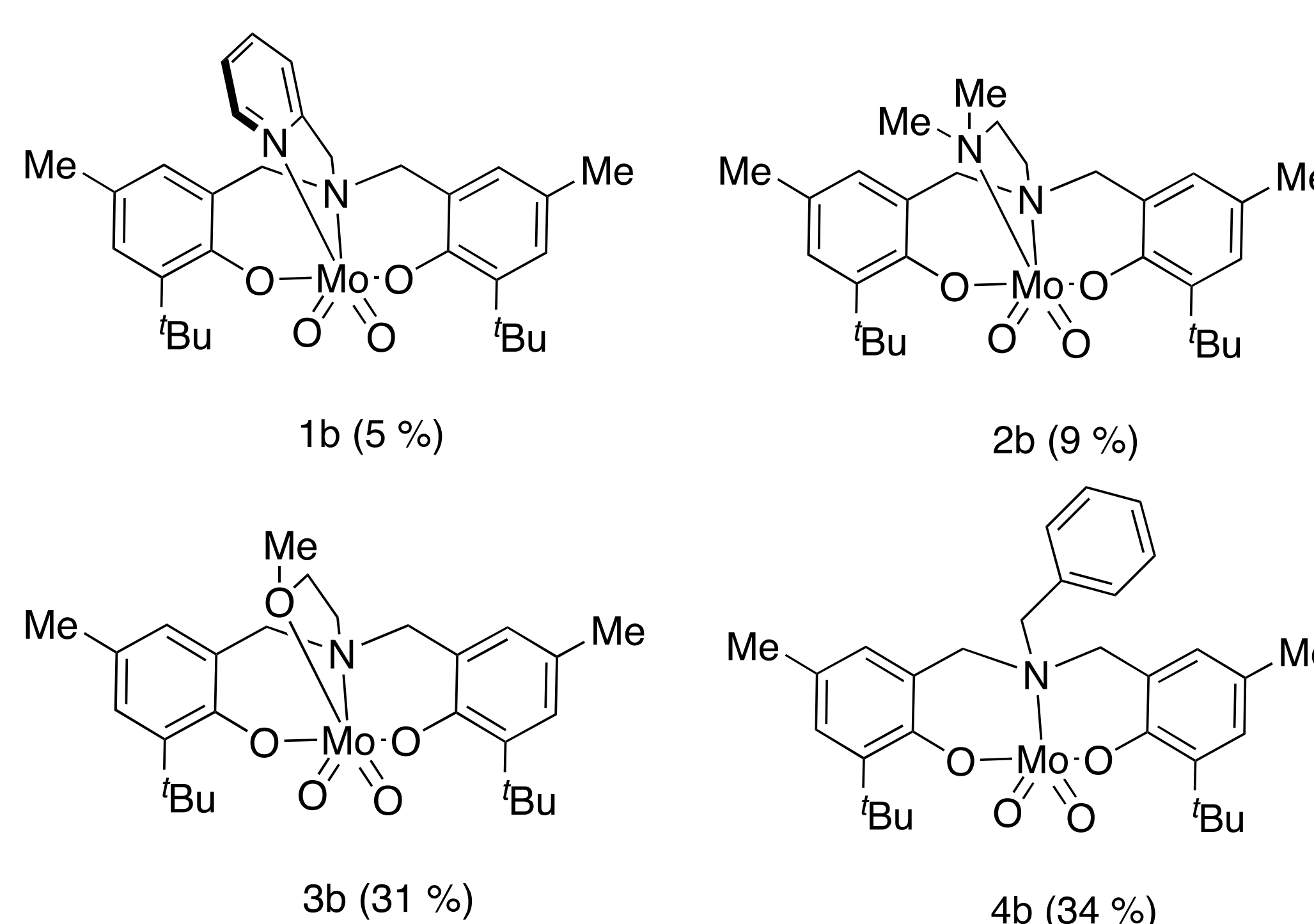
Ligand Synthesis



NMR Spectrum of Ligand and Complex



Catalyst Optimization

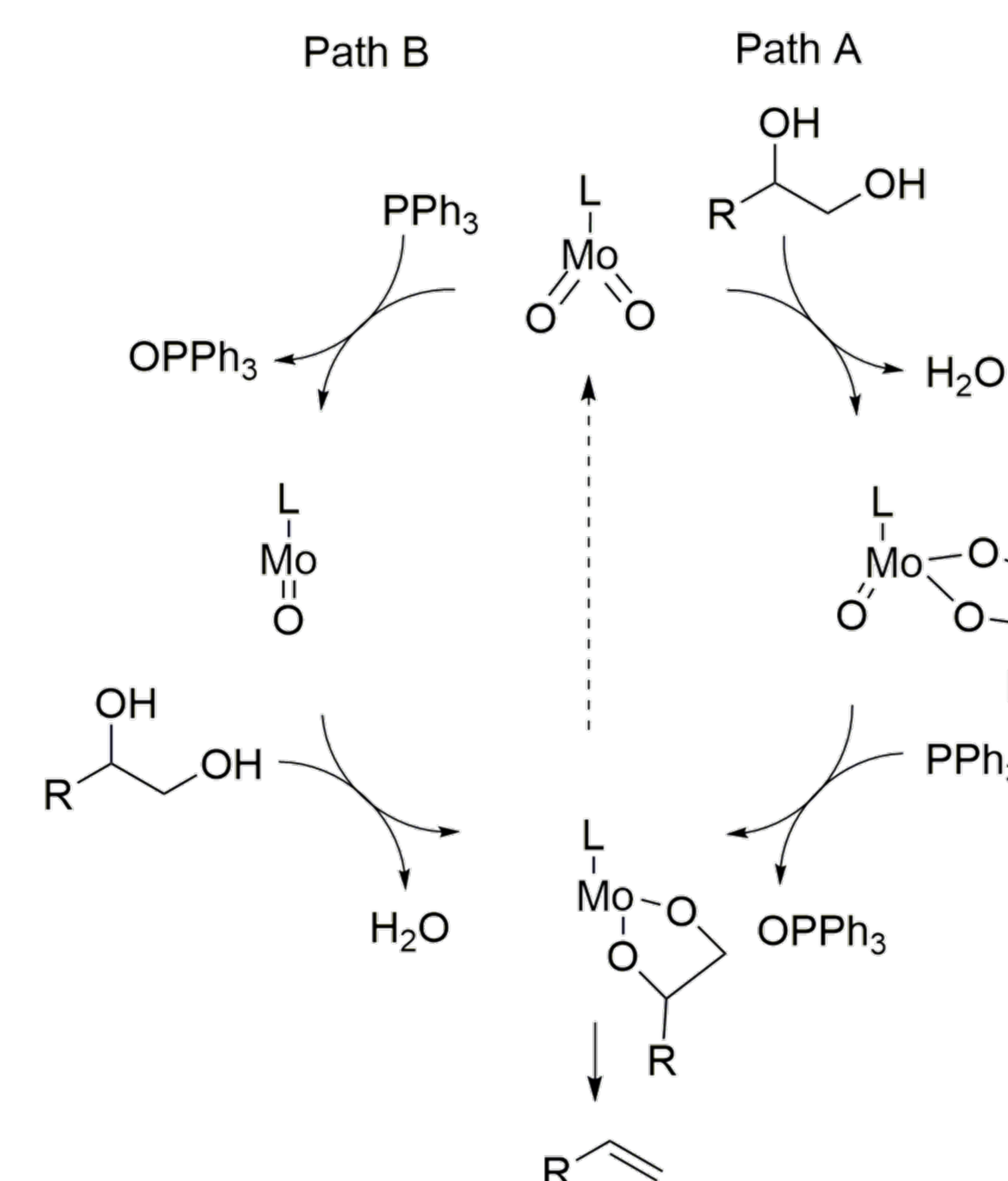


Solvent-Varied DODH Reaction

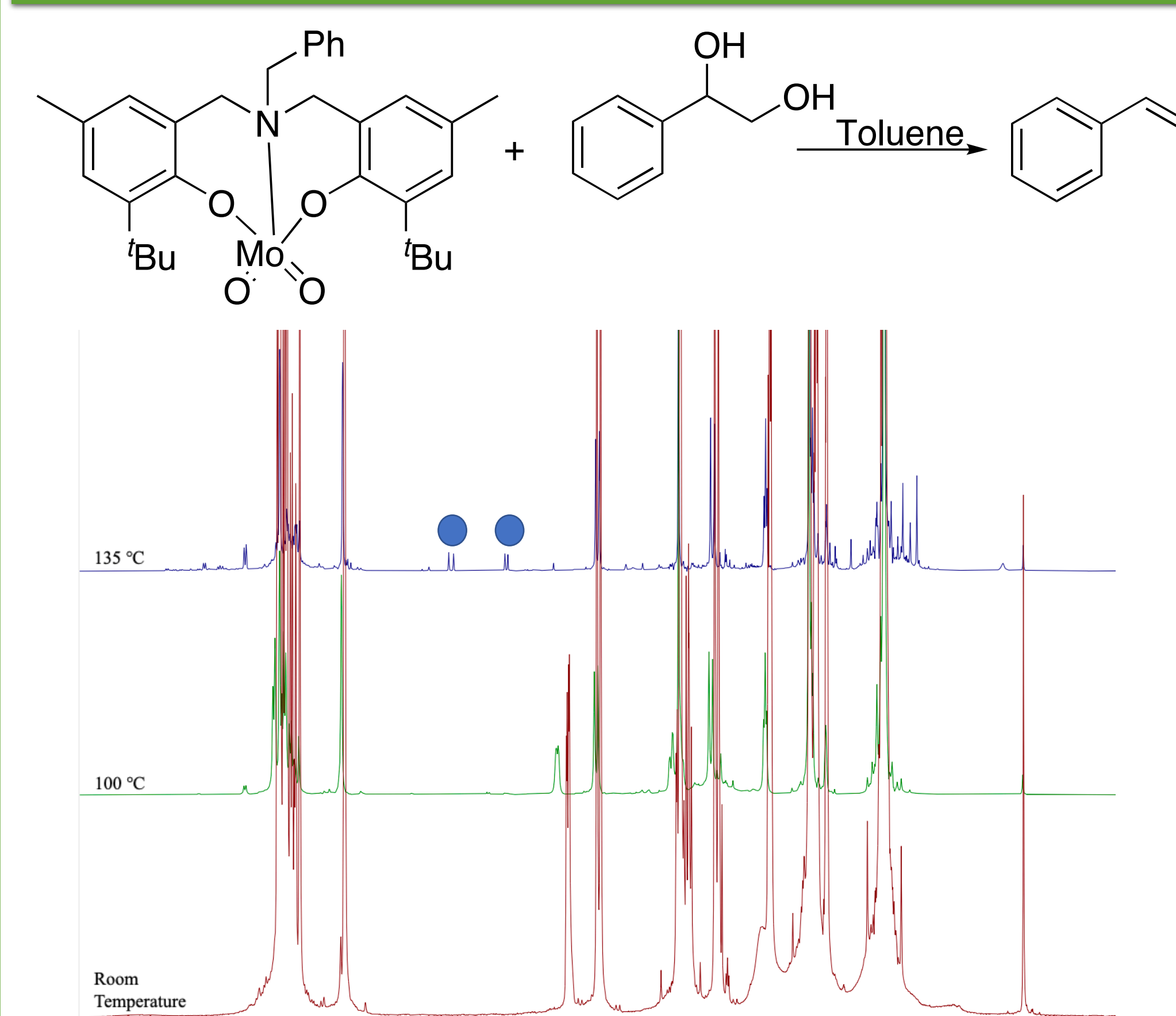
Entry	Catalyst	Solvent	Yield (%)
1		Mesitylene	33
2		Xylene	30
3		Toluene	24
4		Dimethyl Formamide	18
5		Propylene Urea	22
6		Water	No Reaction

*Yield determined by ¹H NMR using 1,3,5-trimethoxybenzene as the internal standard

Proposed DODH Mechanism



DODH Mechanism NMR



Conclusions and Future Work

- The nature of the pendant arm in the complex affects DODH capabilities
- Reaction is dependent upon the polarity of the solvent.
- Explore microwave irradiation methods

Acknowledgements

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