Synthesis of Alternative Fuels using Bimetallic Hydrogen Activation for Clean Energy

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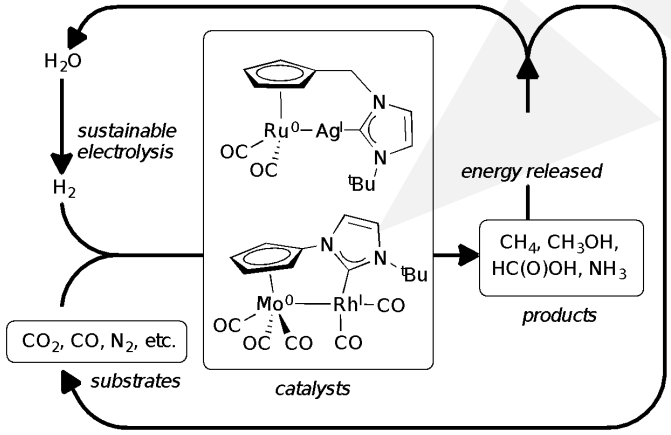
ABSTRACT

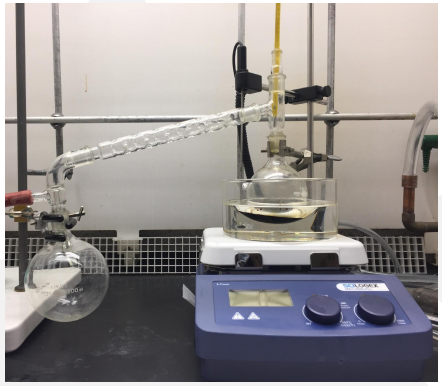
Our project aims to develop catalysts for the conversion of hydrogen gas to carbon-based liquid fuels with high energy density. Our approach involves bimetallic catalysts, supported by bifunctional ligands, which have the potential to break the symmetry of the hydrogen molecule. Oxidative addition of hydrogen across a metal-metal bond is expected to produce a metal hydride complex featuring both a hydridic metal hydride and an acidic metal hydride. We anticipate metal dihydrides of this nature will be poised for the hydrogenation of a carbon source such as carbon dioxide. Here we report the synthesis and NMR characterization of key bifunctional ligand scaffolds and our plans for the preparation of metal complexes with the potential to act as catalysts for the conversion of hydrogen gas to liquid fuels.

BACKGROUND

The ability to store renewable energy in chemical fuels is crucial for the development of a sustainable global energy cycle. Hydrogen gas, produced by the electrolysis of water, is a clean renewable fuel, but has a very low energy density compared to conventional fuels. Our goal is to develop catalysts for the conversion of hydrogen to liquid or liquifiable fuels with high energy density.

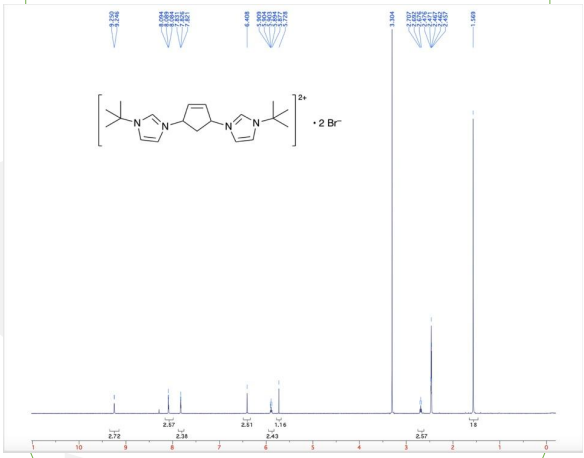


METHODS



The synthesis of 1,4-bis(3-*tert*-butylimidazolium-1-yl) cyclopent-2-ene bromide **2.**

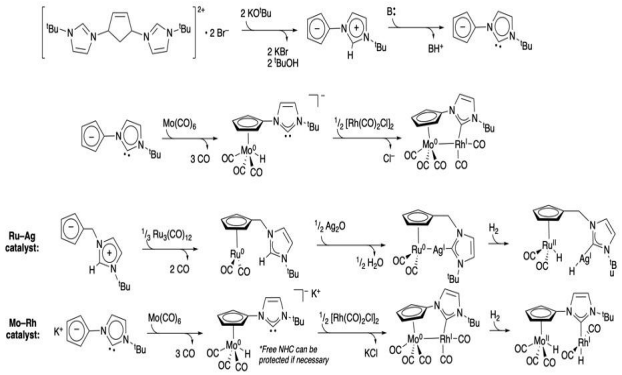
DATA



NMR Spectra for [$CpIm_2$]Br

FUTURE DIRECTIONS

The immediate goal of the project is to complete the synthesis of a bifunctional ligand. Then we plan to investigate the preparation of transition metal complexes such as the molybdenum-rhodium complex shown in the scheme. We anticipate that certain heterobimetallic complexes will be active towards activation of hydrogen for the production of renewable fuels and may serve as catalysts for other useful chemical transformations.



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2. Coleman, K. S.; Turberville, S.; Pascu, S. I.; Green, M. L. H. *Tetrahedron Letters* **2004**, *45*(2004), 8695–8698.

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