Biomimicry: Synthetic Models of an Organometallic Nickel Enzyme
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Synthetic Fuels
Our society's reliance on carbon-based fossil fuels is not sustainable and has a substantial negative impact on our environment. Chemistry plays a vital role in the development of alternatives to fossil fuels.

Clean energy sources such as solar power and wind power are intermittent. We need efficient ways to store renewable energy in chemical fuels or fuel cells so that the energy can be released as needed.

Hydrogen (H2), produced renewable via the electrolysis of water, has the potential to replace fossil fuels. However, hydrogen has low energy density compared to liquid fuels such as petroleum. The goal of our research is to develop catalysts for the conversion of hydrogen to liquid or liquidifiable fuels.

We want to understand biological energy storage on a molecular level and use principles from biological catalysis to develop artificial catalysts for energy storage and the production of renewable fuels.

Lactate Racemase
Lactate racemase is an enzyme whose active site features the only known example of a biological pincer complex. The enzyme catalyzes the interconversion of the two optical isomers of lactic acid.[1]

The cofactor of lactate racemase is an organometallic complex containing a nickel ion coordinated by a pincer ligand and a histidine residue.[2]

The proposed mechanism for lactate racemization involves proton-coupled hydride transfer, an important step in proposed renewable fuel cycles.[3]

We are developing synthetic models of the lactate racemase cofactor in order to study their reactivity and improve our understanding of the mechanism of lactate racemization. Our results could inform the development of catalysts for renewable fuel production.

Results
We have synthesized key precursors to a series of related enzyme models.

The reaction of Compound 1 with refluxing SOCl2 was carried out at 65 °C under an atmosphere of nitrogen, producing Compound 2.[4]

Compound 2 was oxidized by kBrO3 in aqueous solution, resulting in the formation of Compound 3.[5]

The products were isolated by vacuum filtration and characterized by nuclear magnetic resonance (NMR) spectroscopy.

Conclusions
We have demonstrated the synthesis of key precursors to synthetic models of the lactate racemase cofactor. These precursor compounds could serve as the basis for a whole library of enzyme models.

Plans for future research include the investigation of the reactivity of the enzyme models and their catalytic activity in hydride-transfer processes. These studies could include experiments to determine the effects of steric and electronic parameters on reaction rates as well as the optimization of catalytic conditions.

We anticipate this project will shed light on the role of the unique organometallic cofactor of lactate racemase and may inform the design of biomimetic catalysts for related reactions, particularly reactions relevant to hydrogen storage and renewable fuels.

References

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