



Molecular-based technology directly using crude hydrogen



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Abstract

Molecular hydrogen (H_2) is one of the most important energy carriers. In the mid-term future, a huge amount of H_2 will be produced from a variety of hydrocarbon sources through the in-depth purification of a gaseous mixture of H_2 , CO, CO_2 , and other components. However, bypassing these purification processes is desirable, given their energy consumption and environmental impact, which ultimately increases the cost of H_2 . Here, we demonstrate a strategy to separate H_2 from a gaseous mixture of $H_2/CO/CO_2/CH_4$ and simultaneously store it in *N*-heterocyclic compounds that act as liquid organic hydrogen carriers (LOHCs), which can be applied to produce H_2 by subsequent dehydrogenation (Figure). Our results demonstrate that LOHCs can potentially be used for H_2 purification in addition to their well-established use in H_2 storage.

Background & Results

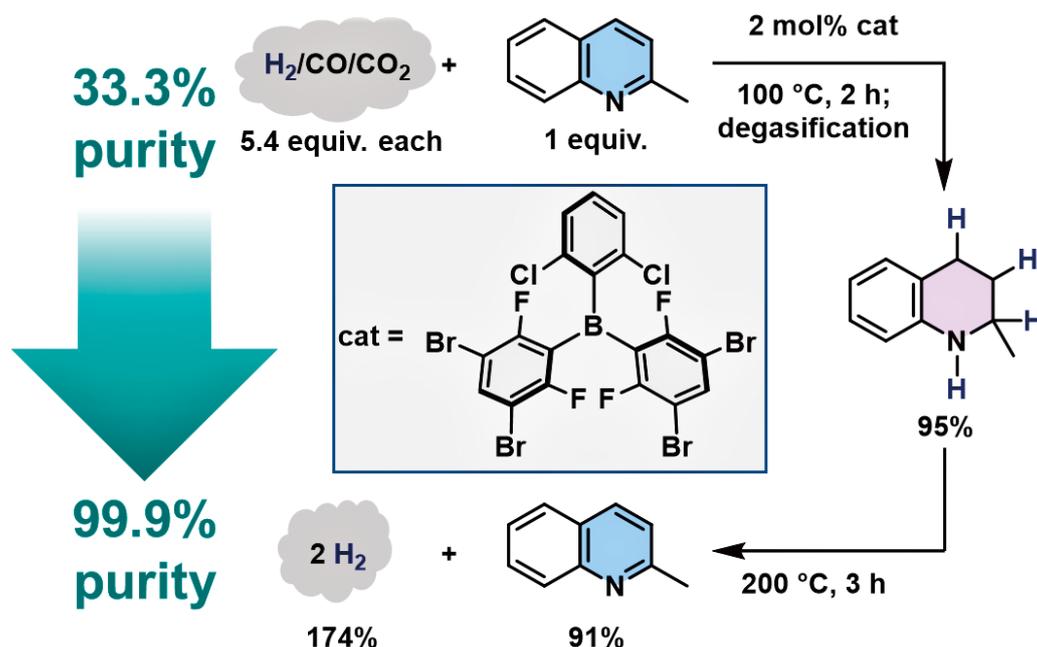
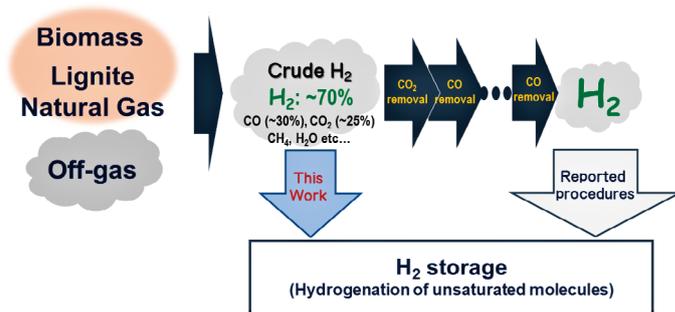
Hydrogen is essential to the modern economy, and expanding its utility in a more sustainable society is a major global priority. A major obstacle to this goal is how we currently produce hydrogen. There are many methods for producing hydrogen—such as by reacting high-temperature steam with natural gas—but these approaches result in the production of crude hydrogen, which contains contaminant gases that are difficult to remove, decreasing the value of the resulting hydrogen. For the commercial use of hydrogen, all contaminants must be rigorously removed by multistep, energy-intensive processes that are independently optimized for each contaminant, making it difficult to extract the hydrogen from the crude mixture containing the by-products. The difficulty of extracting hydrogen from common contaminant gases has restricted

the utility of liquid organic hydrogen carriers, the state-of-the-art for hydrogen storage. In these systems, many researchers have struggled for decades to overcome the challenge of inducing the carriers to uptake—i.e., store—hydrogen in the presence of contaminant gases.

To overcome these challenges, we have synthesized shelf-stable triarylboranes that took up hydrogen even in the presence of common contaminant gases, achieving the following ground-breaking results: hydrogen storage (with up to >99% efficiency) and subsequent hydrogen release at a purity of up to 99.999%.

Significance of the research and Future perspective

This work demonstrated a proof-of-concept for a novel hydrogen production method that eliminates the need for separate purification stages prior to storage, and it thus demonstrates the potential to increase the economic sustainability of hydrogen as an energy carrier.

**Patent** Japanese Patent No. 7079696, Japanese Patent Application No. 2023-95773, No. 2023-185532**Treatise** Hoshimoto, Yoichi et al. Main group catalysis for H_2 purification based on liquid organic hydrogen carriers. *Sci. Adv.* 2022, 8, eade0189. doi: 10.1126/sciadv.ade0189**U R L** <https://www.azom.com/news.aspx?newsID=60330>
<https://newenergyandfuel.com/2022/12/01/proof-of-concept-for-new-hydrogen-production-and-storage/>
<https://cosmosmagazine.com/science/hydrogen-storage-borane/>**Keyword** hydrogen, crude hydrogen, hydrogen storage, hydrogen purification, catalysts