Liquid Organic Hydrogen Carriers for Hydrogen Fuel Storage: Heterocyclic N and O Compound Dehydrogenation Utilizing the Iridium PCP Pincer Catalyst

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Liquid Organic Hydrogen Carriers (LOHCs) are one of the most promising concepts for a new alternative renewable energy source. LOHCs are chemical compounds in which large amounts of hydrogen can be put on and taken off in a continuous cycle. The chemical compounds have this ability because they include stable chemical ring structures with many carbon bonds. Using C-H bond activation, the bonds between the hydrogen and the carbon atoms are broken, allowing the hydrogen gas from the chemical ring structure to be removed. The dehydrogenation reaction results in an unsaturated product where carbon double bonds make up for the loss of the hydrogens. The hydrogen taken from the LOHCs can be used to produce clean energy in Proton Exchange Membrane (PEM) fuel cells. However, no practical substrates for the implementation of LOHCs have been discovered. According to the study conducted by Air Products, the characteristics of the best substrate would be: (1) A fused ring system that is aromatic, (2) The rings incorporate N/O heteroatoms, and (3) Substrates with structures that fuse to a 5-membered ring. All three substrate characteristics will be addressed using various heterocyclic nitrogen and oxygen substrates in order to find a practical substrate. The research will also determine whether incorporating an N heteroatom is more efficient than incorporating an O heteroatom. Ten possible substrates were selected and tested using the acceptor method, with the [Ir]HCl PCP Pincer catalyst and a 1:1 molar ratio of substrate to additive tert-butylethlene (tbe). The experiment tests the ideal substrate characteristics and the ideal method, which has never been done before. Through the research, N-Methylperhydrocarbazole has been identified from the data to be a possible LOHC.

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