Hydrogenation and dehydrogenation of 9-acetylcarbazole as a prototype of a liquid organic hydrogen carrier

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Liquid organic hydrogen carriers (LOHCs) such as carbazole-based compounds have been paid attention as a new type of hydrogen storage materials because of their high hydrogen storage capacity and good reversibility between hydro/dehydrogenation reactions. In addition, they are liquid states with storing hydrogen so that it is possible to be transported by pipeline. In our previous simulation results, it was found that 9-acetylcarbazole has appropriate thermo-physical properties calculated by Density Functional Theory (DFT) and Group-Contribution method. In the present work, hydrogenation reaction of 9-acetylcarbazole, followed by dehydrogenation were performed to verify the simulation results and the capacity of hydrogen storage. Products of each experiment were analyzed by Infrared spectroscopy and Nuclear Magnetic Resonance, which were compared with the vibration analysis calculated by DFT to identify the structure of the products.