Evaluation of *m*-Phenyltoluenes as a New Class of Liquid Organic Hydrogen Carrier Systems

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A concept based on a reversible catalytic hydro-dehydrogenation reactions using liquid organic hydrogen carriers (LOHCs), has been attracting widespread interest in the fields of hydrogen storage and transportation. Although many efforts have been devoted to developing LOHCs, there are a few ideal materials that satisfy the requirements of high hydrogen storage capacity (> 6.5 wt% H_2), good reversibility, low enthalpy of reaction, and being in liquid state. In this work, we suggests the first use of *m*-phenyltoluenes (*m* = 2, 3, and 4) and their ternary eutectic mixture as a new class of LOHCs. These LOHCs exhibited a higher hydrogen storage capacity (6.7 wt% H_2) compared to those of most established LOHC systems, *e.g.*, Benzyltoluene derivatives (6.2 wt% H_2). More interestingly, it was demonstrated that the ternary mixture of *m*PTs showed good reversibility for hydrogenation and dehydrogenation reactions, and a low ternary eutectic point of −19.9 °C. In addition, the enthalpies of dehydrogenation were investigated by density functional theory calculations.