Selective Dehydrogenation of Formic Acid Using an Efficient Cost-Effective Ruthenium-Based Catalyst for Generating Power in Automobiles

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Hydrogen is a promising renewable energy carrier. However, it has the lowest density of all other substances, so it needs to be compressed to run a car. Formic acid (FA) is an attractive liquid candidate to store hydrogen because of its low flammability and high hydrogen density, but the low efficiency and high cost of the catalysts are obstacles to using FA as a hydrogen carrier. Herein, I have synthesized a new cost-effective ruthenium catalyst for use in FA dehydrogenation selectively. The study consists of five main steps: 1- Catalyst synthesis at room temperature and characterization by proton and carbon NMR 2- Performance optimization by solvents screening four solvents (DMSO, toluene, THF, and water) and then measuring the turnover frequency (TOF) under six different sodium formate (SF)/FA ratios 3- Gas composition analysis using a gas-chromatograph thermal conductivity detector (GC-TCD) 4- Determining the overall turnover number (TON) of the system 5- Mechanistic investigation. While the highest TOF achieved was determined to be 2205 h-1 in a 1:1 ratio, the highest yield was 97.14% in a 10:1 mixture of SF/FA. GC-TCD analysis demonstrated superior selectivity of the catalyst as no trace amount of CO was found. The overall stability of the system was determined to be approximately 1400 min and a maximum overall TON of 40,000 was achieved. A mechanism was proposed by detecting the hydride intermediate using proton NMR. These outcomes show potential for the catalyst to contribute to utilizing FA as a hydrogen carrier for power generation, especially automobile applications.

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