Selective Formic Acid Dehydrogenation Under Neat Conditions With Ruthenium-Hydrazine Carboxamide Catalysts

Alangari, Saleh (School: Riyadh School for Boys and Girls)

The high volumetric capacity (53 g H2/L), low toxicity, and ambient stability of formic acid (FA) make it a promising hydrogen carrier, yet efficiently extracting hydrogen in a clean and scalable manner remains a challenge. This research focuses on developing ruthenium-hydrazine carboxamide catalysts for selective FA dehydrogenation under neat conditions, eliminating the need for solvents or additives. Three novel catalysts (Ru-L1, Ru-L2, and Ru-L3) were synthesized, each differentiated by the substitution pattern on their ligands. These ligands were designed, synthesized, and metalated with ruthenium to form the final catalysts, which were fully characterized using ^{1}H-NMR, ^{13}C-NMR, and ESI-MS to confirm their structures and purity. All three catalysts were tested under optimal conditions, where Ru-L3, the methoxy-substituted catalyst, demonstrated the highest efficiency. The focus then shifted toward optimizing Ru-L3, which achieved a TOF of 5,033 h?^{1} and a TON of 1,848 under neat conditions at 92°C with Et3N as the base, significantly outperforming the other catalysts. Gas chromatography analysis verified the selective dehydrogenation of FA, confirming the efficient production of hydrogen. In addition to its high performance, Ru-L3 offers a significant economic advantage, with a cost of $12.58 per mmol, compared to $102–$130 per mmol for iridium-based alternatives, which also require harsh conditions such as DMSO as a solvent at over 100°C. This catalyst presents a low-cost, solvent-free, and scalable solution for hydrogen production, making it a strong candidate for future clean energy applications and industrial hydrogen storage systems.

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