

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

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The high volumetric capacity (53 g H<sub>2</sub>/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 <sup>1</sup>H-NMR, <sup>13</sup>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<sup>-1</sup> and a TON of 1,848 under neat conditions at 92°C with Et<sub>3</sub>N 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.

**Awards Won:**

