CO_2 hydrogenation to liquid fuels and alcohols catalyzed by Ru nanoparticles and molecular Ru complexes

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Abstract

In this work, we present ruthenium nanoparticles (Ru-NPs) and ruthenium molecular complexes (Ru-MCs), both derived from monometallic RuO_2, for directly producing liquid fuels (C_5-C_{22}) and alcohols (C_1-$_{22}$) from CO_2 and H_2. At reaction conditions, RuO_2 undergoes a dynamic transformation into a 'cocktail'-type catalytic system, combining both homogeneous and heterogeneous catalysis corroborated by a detailed suite of characterization techniques. Evidenced by HR-ESI-MS investigations, "hidden" soluble metallic complexes such as $[Ru(CO)_3I_3]^-$ (m/z= 566.61), $[Ru(CO)_2I_3]$- (m/z= 538.61), $[Ru(CO)_2CO_2I_3]^-$ (m/z= 455.70), etc. could be generated in the solution via Ru interaction with ligands, e.g., CO and I which increase in concentration over time according to ICP-OES data. The starting RuO_2 precursor is confirmed by systematic XRD, FTIR, and XPS investigations to show significant changes after exposure to in situ-produced CO, resulting in the formation of catalytically active RuO_xC_y species. The Ru NPs and Ru MCs work in tandem to produce C_5-C_{22} alkanes (54.1 C-mol%) and alcohols (27.1 C-mol%) at a low temperature of 180 ° C with a total pressure of 8 MPa (1:1 of CO_2:H_2) in 14 h. The present research is a crucial mitigation intervention against climate change impact and excessive dependence on fossil fuel resources, as valorization of CO_2 into chemicals and fuels is critically needed in future energy scenarios, especially as sustainable aviation fuels. It further presents an exciting opportunity for advancing the circular bioeconomy system and sustainable chemical development. Additionally, our contribution advances the present limitation of the Ru metal noted for less desirable methane production in CO_2 hydrogenation reactions and further opens novel catalytic routes for monometallic precursors.