Unraveling the hydrogenation of α-ketoglutaric acid on Pd through active sites, substrate structure, and kinetics

Authors & Affiliations

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Highlights

- Production of α-hydroxyglutaric by catalytic hydrogenation of α-ketoglutaric acid
- Identification of 5% Pd/C as the most suitable catalyst for this reaction
- The electronic effect of the α-COOH group compensates for weaker interaction with Pd^0
- Mechanistic proposal by evaluating the reaction kinetics

The bigger picture

The chemical industry has long relied on fossil-based raw materials like coal, oil, and natural gas to produce essential chemicals used in everyday products such as pharmaceuticals and plastics. However, with these resources becoming increasingly scarce and concerns about their environmental impact and potential health risks, there is growing interest in finding more sustainable alternatives. One promising option is biomass, which can be used to produce valuable chemicals in a more environmentally friendly way. A particularly interesting compound in this shift toward sustainable production is α-ketoglutaric acid (α-KGA), which can be made using precision fermentation with various microorganisms and renewable feedstocks. While much of the research has focused on using α-KGA to create different products, one area with significant potential is its conversion into α-hydroxyglutaric acid (α-HGA), a bio-based precursor that could be used in the production of sustainable plastics and other materials.

This study explores a simple, efficient method for producing α-HGA under mild conditions, offering insights into how this conversion process works. The findings not only contribute to the growing body of knowledge around biomass-based chemical production but also provide new avenues for future research aimed at creating more sustainable solutions for industries that depend on fossil resources. By exploring these alternatives, we can work toward reducing our reliance on non-renewable resources and move closer to a more sustainable, circular economy.

Summary

α-Ketoglutaric acid (α-KGA) is an upcoming platform molecule in bio-based industries, with catalytic valorization strategies currently being explored. This study investigates the aqueous-phase hydrogenation of α-KGA using hydrogen gas in a batch reactor, focusing on the role of catalyst properties, substrate structure, and kinetics that affect catalytic activity. 5% Pd/C was the most suitable catalyst (at 40°C and 50 bar) with high turnover frequencies (4.3–7.9 s^{-1}), while other metals (Pt, Rh, Ru, Ni, Cu, and Mo) were inferior. The main product, α-hydroxyglutaric acid, was typically produced in high yield (95%), with minor formation of γ-carboxyl butyrolactone (3%). Furthermore, the α-COOH group in the substrate enhanced the activity on Pd whereas inhibition occurred on oxophilic Ru. Finally, a two-step addition of hydrogen to α-KGA on Pd emerged as the most plausible surface reaction pathway. These findings provide a thorough understanding of aqueous-phase hydrogenation of activated α-ketoacids, which is useful for other biomass-derived oxygenates.

Graphical abstract