



Research Paper

Precursor-driven acidity enhancement in Titania-modified KCC-1 for efficient n-Hexane hydroisomerization

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ABSTRACT

The catalytic activity of titania-loaded fibrous silica (KCC-1) catalysts synthesized using different titania (Ti) precursor compounds was first explored for the hydroisomerization of n-hexane. The Ti crystallite sizes reveal a descending order: TiSO₄/KCC-1 (9.70 nm) > Ti-Iso/KCC-1 (4.86 nm) > TiCl₄/KCC-1 (3.64 nm), indicating the lower Ti distribution for TiSO₄/KCC-1. A decline in surface area is observed as Ti-Iso/KCC-1 (549 m² g⁻¹) < TiSO₄/KCC-1 (599 m² g⁻¹) < TiCl₄/KCC-1 (619 m² g⁻¹) < KCC-1 (644 m² g⁻¹), resulted from partial blockage of TiO₂ particles and structural disruption of KCC-1 support. The NH₃-TPD analysis reveals the total area acid amount of Ti-Iso/KCC-1 surpassed the other Ti-loaded KCC-1 catalysts, attributed to the presence of acidic protons on isopropoxide ligands. Among the n-hexane hydroisomerization catalysts, Ti-Iso/KCC-1 stands out with the most substantial isomer production, achieving a notable 59.7 % yield, followed by TiCl₄/KCC-1 (54.5 %) > TiSO₄/KCC-1 (54.1 %) > KCC-1 (23.1 %). This trend corresponds with the sequence of total area acid amount from NH₃-TPD desorption peaks, highlighting the enhanced isomer activity in Ti-Iso/KCC-1 compared to others due to higher amounts of acidity.

1.0. Introduction

Straight-chain hydrocarbons are crucial to transportation fuels like diesel, gasoline, and jet fuel, but their prevalence in crude oil poses environmental challenges, affecting combustion and engine efficiency. Indeed, the stringent requirements for reducing aromatic hydrocarbon content in commercial gasoline have prompted a focused exploration of the isomerization pathway [1–3]. Remarkably, the isomerization approach selectively rearranges hydrocarbon molecules to enhance fuel octane ratings, aligning with the pursuit of cleaner and more efficient energy sources [4–6]. For example, n-hexane has a lower Research Octane Number (RON) of 24.8, while its branched isomers, such as 2-methyl pentane (RON 73) and 2,3-dimethyl butane (RON 101), showcase the potential for improved combustion efficiency reduced knocking, and enhanced fuel quality through isomerization [7]. Indeed,

the branched isomers are more stable and reactive, making them more efficient feedstocks for downstream reactions. The isomerization process can thus increase the yield of valuable products like aromatics, which are key intermediates in the production of polymers, plastics, and other chemicals.

Hydroisomerization, which converts n-hexane into more branched isomers using hydrogen, typically relies on bifunctional metal-acid catalysts. The active metal sites initiate hydrogenation/dehydrogenation reactions, and the support's acidity facilitates the isomerization pathway, promoting the formation of preferred branched hydrocarbon structures. Thus, the choice of catalyst for n-hexane hydroisomerization is a critical determinant in dictating the catalyst efficiency and product selectivity. Active metals from noble metals like platinum (Pt) and palladium (Pd) are frequently utilized for their well-established catalytic activity in bifunctional catalysts for n-hexane hydroisomerization [8,9].

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