

A comprehensive study of indole catalytic hydrodenitrogenation under hydrothermal conditions

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July 13, 2021

Abstract

This article focuses on the catalytic hydrodenitrogenation (HDN) mechanism of indole under hydrothermal conditions. Both gaseous hydrogen and liquid hydrogen donor formic acid (FA) can improve indole conversion and total yield of denitrogenated products. Ru/C showed the highest activity among the catalysts for indole conversion in all temperature conditions with the existence of H₂ and 91.17 % indole was converted at 400 °C and 60 min. Based on reaction kinetic experiments, a kinetic model was developed to describe the hydrothermal HDN reaction of indole over the home-made Ni₈₀Ru₂₀/γ-Al₂O₃ catalyst, which clearly captured all data trends and fitted the temporal variation of all major liquid products. High activation energy for formation of O-containing substance o-cresol from both mathematical fitting and density functional theory (DFT) calculation indicated a rare occurrence of reaction between pyrrole ring-opening product methyl aniline and H₂O, consistent with experimental observation that only a trace of o-cresol was detected.

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