催化、动力学与反应器

CO₂-高温液态水介质中的频那醇重排反应

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摘要 提出了一种通过引入 CO_2 来提高高温液态水中频那醇重排反应速度的方法,测定了不同 CO_2 初始压力和温度等对频那醇重排反应动力学的影响。实验结果表明: CO_2 的引入可以提高高温液态水中频那醇重排反应的速度及产物频那酮的收率。不加 CO_2 时频那醇重排反应的活化能为81.1 kJ·mol⁻¹, CO_2 初始压力为0.2 MPa时的活化能为87.1 kJ·mol⁻¹,二者差别不大。通过对气、液相产物的分析,确认了主要的副产物为2,3-二甲基-1,3-丁二烯,并对其反应机理进行了探讨。该方法具有环境友好的特点。关键词

高温液态水 二氧化碳 重排反应 频那醇 频那酮

分类号

Pinacol rearrangement in CO₂ enriched high temperature liquid water

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Abstract

An environmentally benign method to accelerate the pinacol rearrangement in high temperature liquid water by the addition of CO_2 was proposed. The effects of CO_2 initial pressure and temperature on the kinetics of pinacol rearrangement were studied. The experimental results showed that the reaction rate could be greatly increased with the addition of CO_2 . The activation energies evaluated were 81.1 kJ·mol⁻¹ without CO_2 , and 87.1 kJ·mol⁻¹ with CO_2 initial pressure at 0.2 MPa, which showed no significant difference. The main by-product was confirmed to be 2,3-dimethyl-3-butadiene by GC/MS and the possible reaction mechanism was proposed.

Key words

high temperature liquid water CO2- rearrangement pinacol pinacolone

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