

Mechanism on Redistribution Synthesis of Dichlorodimethylsilane by $\text{AlCl}_3/\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ Core-shell Catalyst

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Abstract

The redistribution method plays an important role in addressing the issue of organosilicon by-product in the direct synthesis of dichlorodimethylsilane, and the redistribution mechanism is still a topic of debate. The redistribution by $\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ core-shell catalyst and post-modified $\text{AlCl}_3/\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ catalyst was technically performed using the Density Functional Theory (DFT) at the level of B3LYP/6-311++G(3df,2pd). The result shows that No.1 active site of $\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ core-shell structure has a significant effect on the activity of the catalyst. Indicating that the active center involved in the reaction is H provided by Al-O-H bond, which is an obvious catalytic active center of Bronsted acid. Furthermore, post-modified $\text{AlCl}_3/\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ catalyst is in more favor of redistribution reaction comparing with $\text{ZSM-5(3T)}@ \gamma\text{-Al}_2\text{O}_3$ core-shell catalyst. It ascribes to the robust Lewis site of aluminum chloride favorable modification.

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