Critical Role of Microporous Structures in Catalysts for Side-Chain Alkylation of Toluene to Styrene

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In this study, the effects of acid-base properties and microporous structures of zeolite catalysts on side-chain alkylation of toluene with methanol were comprehensively investigated. Our results revealed a significant dilemma in the design of catalyst for this reaction. The main active sites required for side-chain alkylation of toluene are base sites. However, the catalysts having sufficient basicity have limited Lewis acidity, which is ineffective for stabilizing toluene under elevated temperatures. Fortunately, the microporous structure of zeolites provides additional secondary interactions (e.g., van der Waals interaction) to toluene, which remarkably increases the catalytic activities of basic zeolites. In contrast, the model catalysts synthesized using mesoporous A zeolite showed no toluene adsorption at all due to the absence of any accessible microporosity. Consequently, the A zeolite catalysts which have similar acid-base properties to those of the X zeolite catalysts showed no detectable toluene alkylation activity. The results clearly showed the importance of secondary interactions (or solvation effects) in zeolite catalysis for toluene side-chain alkylation.