

Mechanistic Insights into the Zeolite-Catalyzed Isomerization and Disproportionation of *m*-Xylene

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The mechanisms of *m*-xylene isomerization and disproportionation over thirteen medium-pore zeolites and three large-pore ones are investigated. H-TNU-10 and H-ZSM-57 with intersecting 10- and 8-ring channels were found to show considerably higher *p/o*-xylene and isomerization/disproportionation ratios than H-ZSM-5, a commercial *m*-xylene isomerization catalyst. The GC-MS results from used zeolite catalysts demonstrate the intrazeolitic build-up of tri- and tetramethylated diphenylmethane species, whose existence during the *m*-xylene transformation over any acidic catalyst has not been experimentally verified until now. These bicyclic aromatic compounds were ascertained to serve as reaction intermediates of bimolecular *m*-xylene isomerization within the micropores not only of large-pore zeolites but also of medium-pore materials at temperatures lower than 250 °C or so, once there are internal void spaces larger than 10-rings. The overall GC-MS results of our work demonstrate that transition state and product shape selectivities are experimentally distinguishable from each other.