

Selective Formation of Pentamethyl Diphenylmethane Reaction intermediates during 1,2,4-Trimethylbenzene Disproportionation over Large-Pore Zeolite Y: A Theoretical Investigation

변영철¹, 차승혁^{2,1}, 홍석봉^{2,1,*}¹포항공과대학교; ²나노다공성재료합성연구단
(sbhong@postech.ac.kr*)

1,2,4-trimethylbenzene (TMB) disproportionation has long been considered as one of the potential technologies for the production of p-xylene. Very recently, our group has demonstrated that pentamethyl diphenylmethane (pmDPM) species act as real reaction intermediates of the 1,2,4-TMB disproportionation over the large-pore zeolite LaNa-Y. It was also found that only six isomers out of nine possible ones are generated inside the pore of zeolite LaNa-Y. In this study, the potential energy levels of the formation of all nine pmDPM isomers were determined by density functional theory calculations in order to more precisely investigate the effect of zeolitic pore structure. Our theoretical calculations reveal that 2,2',3,4',6-, 2,2',3,5',6-, and 2,3',3,4',6-pmDPMs, which were not detectable by GC-MS analysis of the used LaNa-Y catalysts have much higher energy levels than those of other six isomers. This strongly suggests that the formation of particular pmDPM isomers is highly influenced by the zeolitic pore structure, which can be considered as an indirect evidence for the transition-state shape selectivity.