Syngas Conversion beyond Chemical Equilibrium by an *in situ* Bimolecular Reaction

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Syngas, which can be generated from petroleum alternatives such as coal, natural gas (including shale gas), and biomass, is a versatile intermediate for fuels and value-added products such as light olefins and oxygenates. The conversion of syngas to methanol is limited by the equilibrium that requires high pressure and low temperature for high per-pass conversion. In this study, a bimolecular reaction between toluene and methanol formed *in situ* was tested over bifunctional catalysts under a moderate pressure of 30 bar. In the *in situ* methylation of toluene using syngas, the CO conversion rate was increased by about ten times compared with that over monofunctional methanol synthesis catalyst mainly due to the displacement of equilibrium. To further elucidate the fundamental catalytic behavior underlying the complicated in situ methylation, we report herein asystematic study on the *in situ* methylation of toluene using syngas on a bifunctional mixture of Cr_2O_3/ZnO (CrZ) and HZSM-5 catalysts.