Supporting Information

Surface Silanol Sites in Mesoporous MFI Zeolites for Catalytic Beckmann Rearrangement

Hanyoung Park,^{a,b} Jisuk Bang,^{a,b} Hongjun Park,^b Jaeheon Kim,^b Jeong-Chul Kim,^b Jeong Young Park^{*,a,b} and Ryong Ryoo^{*,c}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 34141, Republic of Korea
^b Center for Nanomaterials and Chemical Reactions, Institute for Basic Science (IBS), Daejeon, 34141, Republic of Korea
^c Department of Energy Engineering, Korea Institute of Energy Technology (KENTECH),

Naju, Jeonnam 58330, Republic of Korea

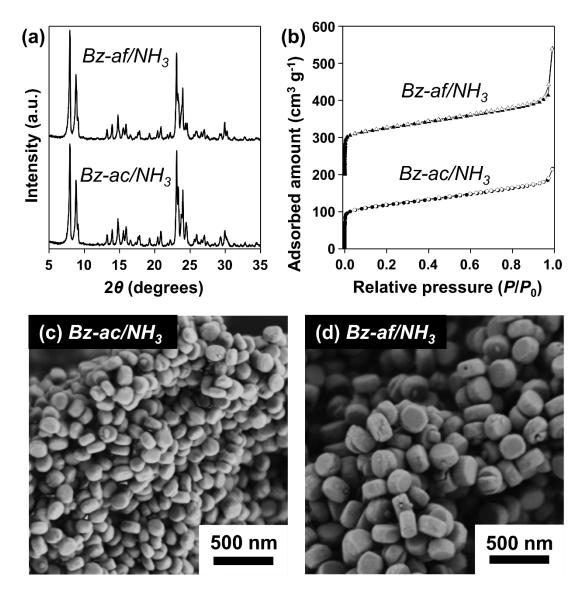


Fig. S1. Characterization of Bz- ac/NH_3 and Bz- af/NH_3 samples: (a) XRD patterns, (b) Ar adsorption isotherms, and SEM images of (c) Bz- ac/NH_3 and (d) Bz- af/NH_3 . The isotherms were offset vertically by 200 cm³ g⁻¹ STP.

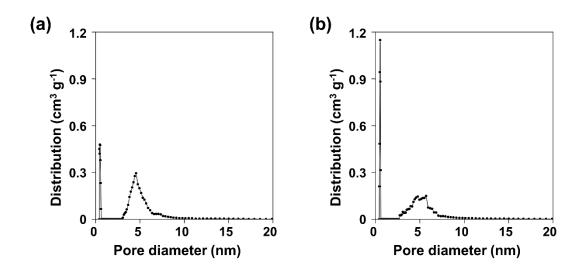


Fig. S2. Pore size distributions of (a)*Mz-ac* and (b) *Mz-af*, calculated by non-linear density functional theory method.

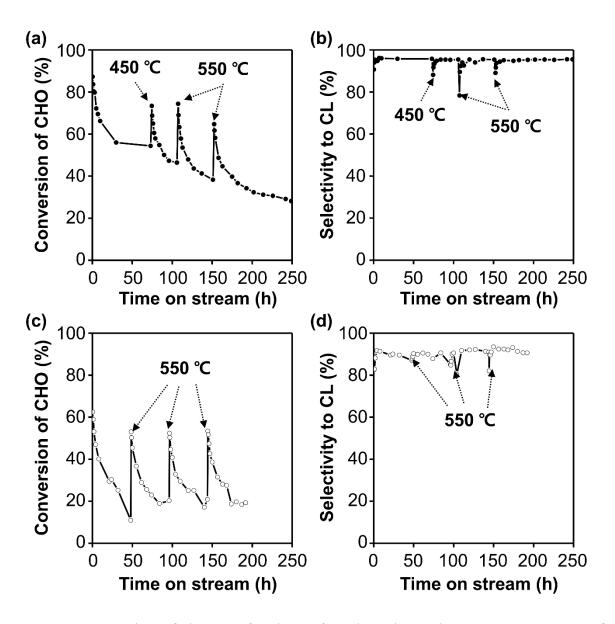


Fig. S3. Regeneration of the *Mz-af* and *Bz-af* catalysts in Beckmann rearrangement of cyclohexanone oxime (CHO). (a) Conversion of CHO and (b) selectivity to ε -caprolactam (CL) over *Mz-af* as a function of the time-on-stream. (c) CHO conversion and (d) CL selectivity over *Bz-af*. Reaction conditions: 0.884 M oxime in ethanol; WHSV = 3.4 h⁻¹; temp = 350 °C; N₂ flow rate = 15 cm³ min⁻¹. The catalysts were heated in an air flow (flow rate: 50 cm³ min⁻¹) for their regeneration at the denoted temperatures, and then cooled down to the reaction temperature.