A Study on the Knoevenagel Condensation Reactivity Through Functional Group Modulation of Metal–Organic Frameworks (MOFs)

Yune, Nayoung (School: Daegu-il Science High School)
Kwon, Minju (School: Daegu-il Science High School)
Kang, Hyewon (School: Daegu-il Science High School)

This study aimed to address the recovery and reusability limitations of conventional homogeneous catalysts. For this purpose, zirconium-based metal–organic frameworks (MOFs) were synthesized. UiO-66 and four functionalized derivatives (–NH2, –NO2, –OH, and –SO3H) were prepared. These materials were applied as heterogeneous catalysts in the Knoevenagel condensation. The Knoevenagel condensation is a widely used carbon–carbon bond-forming reaction in organic synthesis. It was selected as a model reaction to evaluate recyclable MOF-based catalysts. The structural stability of the synthesized MOFs was confirmed by PXRD analysis. The reaction between benzaldehyde and malononitrile was monitored by ^{1}H NMR spectroscopy, and conversion was evaluated. The –NH2-functionalized derivative showed over 90% conversion at 50 °C and excellent recyclability, demonstrating performance similar to that reported in previous studies. The –NO2-functionalized derivative also exhibited relatively high activity. This result suggests enhanced aldehyde activation through increased Lewis acidity. In contrast, the –SO3H-functionalized derivative showed relatively low conversion under the reaction conditions used in this study. These results indicate that the catalytic performance of MOFs can be tuned by controlling their local chemical environment. This study provided foundational data for the design of sustainable MOF-based catalysts.

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