

The mechanism of Friedlander reaction was investigated theoretically. The main objective was to find a reaction path of Friedlander reaction catalyzed by $\text{Cu}_3(\text{BTC})_2$ (BTC = benzene-1,3,5-tricarboxylic acid), a microporous metal organic framework. In addition, possible mechanisms of non-catalyzed and acid-catalyzed reaction were investigated in the gas phase and in the solution. The suitability of $\text{Cu}_3(\text{BTC})_2$ as catalyst for Friedlander reaction is discussed based on the computational results obtained.