

Amino acids/KI as natural bi-functional catalyst for cyclic carbonate synthesis: A DFT assisted mechanistic approach

Kuruppathparambil Roshan Roshith, 김보미, 박대원*

부산대학교

(dwpark@pusan.ac.kr*)

Naturally occurring amino acids (AA) were identified as efficient co-catalysts for alkali metal halide (MX) mediated synthesis of cyclic carbonates from CO₂ and epoxides under mild reaction conditions of 1 MPa and 120 °C in 3 h under solvent free conditions. The bi-functional system of histidine/KI procured an appreciable TON of 535 for propylene oxide and the detailed studies done with a variety of amino acids revealed that, the basic amino acids afford better conversion rates. The formation of a seven membered ring by the zwitter ionic ends of the amino acid and KI and the epoxide was considered to accelerate the catalysis rate. Quantum mechanical studies using density functional theory were applied to have more insight into the mechanism behind the catalysis. The iodide ions of the MX displayed excellent synergism with the hydrogen bonding groups of the amino acids in the production of cyclic carbonates whereas the bromide and chloride anions were found to have lesser synergistic abilities in the context of cyclic carbonate synthesis.