Cu/Zr binary metal organic frameworks: Heterogeneous catalysts for the efficient solvent-free CO_2 fixation via cyclic carbonates synthesis

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Anthropogenic emission of waste CO_2 gas has reached frightening levels in the biosphere, and is suspected to be causing global warming. Thus, the development of CO_2 capture and sequestration/storage technologies that involve catalyst-mediated reactions such as CO_2 capture, transportation, and storage is essential. MOFs are a new and emerging class of porous material that have been dynamically investigated as catalysts for the synthesis of cyclic carbonates owing to its greater CO_2 affinity. In this study, binary MOFs with HKUST-1 and UiO-66 have been synthesized using solvothermal method. The synthesized binary MOF is investigated for its catalytic efficacy in the synthesis of cyclic carbonates from epoxides and CO_2. The UiO-66/Cu-BTC binary MOF provides high conversion rates of epoxides to cyclic carbonates with >99% selectivity. The appreciable conversion of ECH with the UiO-66/Cu-BTC/TBAB system was influenced by the synergistic effect of the Cu and Zr metals and the Br ion from TBAB. Based on our previous DFT studies and experimental inferences, a plausible reaction mechanism for the binary MOF-catalyzed epoxide-CO_2 cycloaddition reaction was proposed.