Zirconium based metal organic Framework for the CO₂ fixation reactions via cyclic carbonate synthesis

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 CO_2 fixation catalysis is an important and challenging subject in connection with the development of a truly environmentally benign process, because there are many possibilities for CO_2 to be used as a nontoxic, non-flammable and abundant C1 building block. Synthesis of five membered cyclic carbonates from CO_2 and epoxide is 100% atom economical and an ideal representative for its transformation. Metal organic frameworks (MOFs) are crystalline organic–inorganic hybrid structures comprised of metal ions or clusters and multidentate organic linkers connected to metal nodes in one–, two–, or three–dimensional networks. In this work, MOF–802 [$Zr_6O_4(OH)_4(PZDC)_5(HCOO)_2(H2O)$ 2], a microporous metal organic framework has been synthesized and characterized for its crystallinity and textural properties using various physicochemical techniques. Cycloaddition reactions were carried out under mild reaction conditions by using propylene oxide as substrate along with tertiary butyl ammonium bromide co–catalysts. The effect of various reaction parameters such as the catalyst loading, temperature, CO_2 pressure, and time were evaluated. A plausible reaction mechanism also was proposed.