A computational insight into the organic base catalyzed cycloaddition of CO_2 and epoxides

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The ever expanding levels of CO_2 in the atmosphere as well as its potential capability to replace the currently employed C1 feedstocks such as $COCl_2$ and CO, boomed strenuous input in CO_2 conversion research. Herein our work, the common organic bases such as imidazole and pyridine were found as moderately efficient catalysts, but with small amounts of water, the catalysis was accelerated multifold. By employing DFT calculations using B3LYP functionals, the energy and intermediates associated with the imidazole and pyridine catalyzed CO_2-propylene oxide cycloaddition was investigated. With small amounts of water in the system, a pyridine-water-CO_2 adduct, probably a bicarbonate ion is supposedly formed and serves the key role in the catalysis. To verify this possibility, acetate ion is also investigated using computational calculations and results supplemented the proposal that, in case of a pyridine-water catalyst system, with the aid of CO_2, a pyridinium bicarbonate complex is formed and is the main catalytic species for evenutating the cyclic carbonate synthesis.