Organocatalysts containing hydroxyl and amine groups for the cycloaddition of CO_2 and alkyl oxide

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Substantial CO_2 emissions from the massive consumption of fossil fuels have brought about global warming and climate change [1]. This can be decreased by using waste CO_2 as low-cost alternative raw materials in the chemical processes [2]. Of all the possible conversions of CO_2 to C1 or higher-carbon chemicals using molecular catalysts, the most promising reaction in terms of market needs, catalyst performance, and reusability might be the formation of cyclic carbonates by reacting CO_2 with epoxides [3].

The use of CO_2 as a chemical feedstock can be realized by designing a suitable catalyst. An environmentally friendly organic catalyst that does not contain metals or halogens could be favorable for developing inexpensive, sustainable, and green processes. In essence, organocatalysts act as nucleophiles in the synthesis of cyclic carbonates by opening the epoxide ring prior to the addition of CO_2 and subsequent cyclization [4]. Alkanolamines, commonly used as CO_2 scrubbers, were first applied to catalyze the insertion of CO_2 into epoxides, generating cyclic carbonates [5]. In this work, we designed and prepared metal- and halide-free multifunctional alkanolamines for the production of alkyl carbonates to achieve a more environmentally friendly and higher performance catalyst for CO_2 conversion than other organocatalysts. Furthermore, the synergetic effects of amines and hydroxyl groups were also studied.

The oraganocatalysts, bis (methylpiperazinyl) triol were synthesized in a one-step, low-temperature reaction. A reaction mechanism was proposed based on the synergetic effects between the hydroxyl and amine groups. The hydroxyl group of the bis (methylpiperazinyl) triol forms a hydrogen bond with the epoxide oxygen. Therefore, it becomes easier for the epoxide to participate in ring-opening reactions, while the lone-pair electrons on the nitrogen atom of the catalyst activate CO_2 by nucleophilic attack [5].

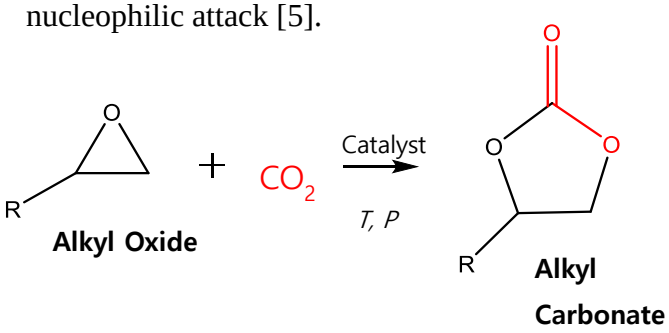

Fig. 1. Catalytic conversion of alkyl carbonate from CO_2 and alkyl oxide.

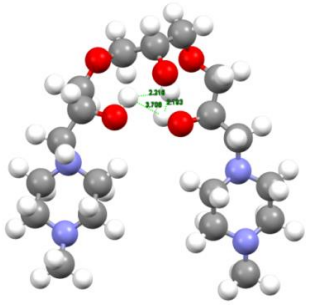

Fig. 2 Bis (methylpiperazinyl) triol multifunctional catalyst for CO_2 cycloaddition reaction.

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