Understanding the catalytic carbonylation of epoxides for the valorization of carbon monoxide

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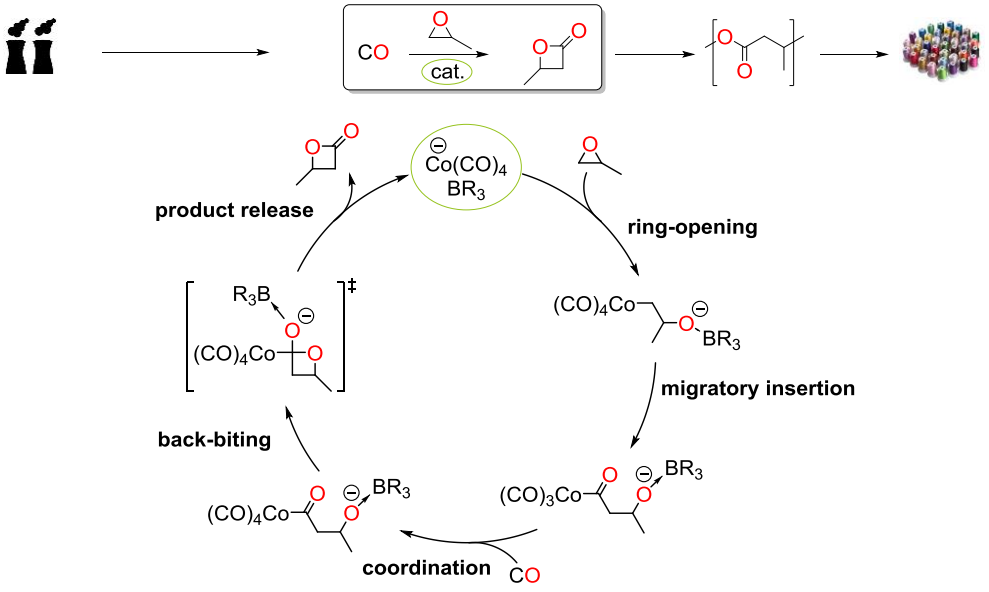
Small molecules released as gaseous wastes by the industries, such as CO and CO2, are attractive C1 building blocks for the production of chemicals. They can indeed reduce our dependence on fossil feedstocks. The catalytic insertion of carbon dioxide into epoxides has been developed over the last decades for the production of cyclic and polymeric carbonates, with industrial success.[1]

The same strategy can be used for the production of polyester from epoxides and carbon monoxide, possibly released from the production of steel.

The catalytic carbonylation of epoxides with gaseous CO leads to β-lactones and this reaction has attracted a particular attention over the past few years. Yet, only few catalytic systems have been developed, all containing a cobalt carbonyl complex assisted by a Lewis acid.[2,3,4,5]

Herein, we disclose a theoretical study to understand the mechanism[6] of carbonylation of epoxides using a cobalt catalyst with Lewis acids. The influence of the Lewis acidy on the activity was investigated through various boron compounds. The DFT calculations, linked with a Lewis acidity scale, can thus be used as a guide for the development of a novel catalytic system.



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