



# 16<sup>th</sup> INTERNATIONAL CONFERENCE ON CARBON DIOXIDE UTILIZATION

## High-throughput screening of catalysts for the co-polymerization of CO<sub>2</sub> and cyclohexene oxide

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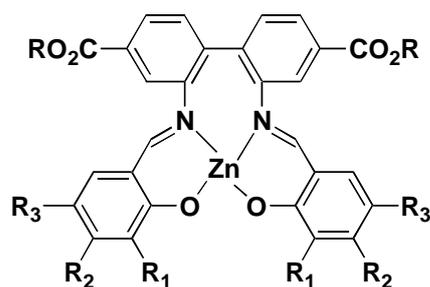
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Heterogenization of homogeneous catalysts often improves the economic and environmental profiles of chemical processes by eliminating the costs and wastes associated with recovery or loss of the homogeneous version. One strategy to immobilize homogeneous catalysts is to incorporate them as linkers in metal-organic frameworks (MOFs).

We have designed and synthesized a set of bis(salicylaldimine) zinc-based catalysts for the co-polymerization of epoxides and CO<sub>2</sub>, that can in principle be incorporated into a MOF post-synthetically. These catalysts are shown in Figure 1.

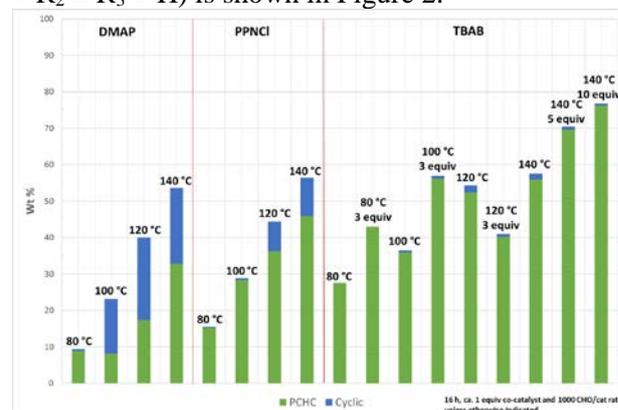


### Bis(salicylaldimine) Zn complexes

**Figure 1.** New zinc catalysts for the co-polymerization of epoxides and CO<sub>2</sub>.

10 different variations of these catalysts, with substituents of varying steric and electronic factors in the R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> positions, have been synthesized. Prior to MOF incorporation, the activity of these catalysts toward the co-polymerization of CO<sub>2</sub> and cyclohexene oxide was screened with high-throughput (HT) techniques. The screening was conducted at four different temperatures (80, 100, 120 and 140 °C) and with four different co-catalysts

(dimethylaminopyridine (DMAP), PPNCI, tetrabutylammonium bromide (TBAB) and excess TBAB). No activity was observed without co-catalyst. The activity of the catalysts for production of both oligomeric polycarbonates and cyclic carbonates was determined by NMR. A representative data set for the parent compound (R<sub>1</sub> = R<sub>2</sub> = R<sub>3</sub> = H) is shown in Figure 2.



**Figure 2.** Catalytic activity of the parent catalyst.

This presentation will discuss the effects of the variations in substituent sterics and electronics, nature of the co-catalyst and reaction conditions on the overall activity and the selectivity to either oligomer or cyclic carbonate, as explored from multi-variate analysis of the data set and the activity comparisons between the HT screening studies and autoclave reactor studies.

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