Proline-based catalyst for CO2/epoxid copolymerisation

Despite its relatively high costs polycarbonates are in many cases the first choice if high quality synthetics are needed. Scientists from the Georg August University in Göttingen developed a highly active catalyst, which allows for the synthesis of polycarbonates out of CO_2 under simple reaction conditions. Thus the technology allows a cost saving production of polycarbonates, while binding CO_2.

Challenge

Even though the production costs are comparatively high, the demand for polycarbonates constantly increases. Its excellent mechanical and optical properties, the suitability for coatings and other surface modifications and its potential for CO_2 capture and storage makes the synthesis of polycarbonates from CO2 highly attractive.
As a result great efforts have been devoted to the catalytic copolymerization of CO_2 with epoxides to form polycarbonates, since the initial discovery by Inoue et al. In 1969. However, activating CO_2 is still a challenge. Ring-opening-polymerization proved to be a suitable strategy for which various promising catalysts have already been developed. Although some proved to be active at the most desirable pressure of one atmosphere in CO_2, they have several drawbacks, which are for example low chemoselectivity, the use of toxic metals and additives, low TON and TOF values and low catalyst isolation yields.

Our Solution

Scientists from the University of Goettingen developed a highly active and readily accessible proline-based dizinc-catalyst for CO_2 / Epoxide Copolymerization. This novel chiral zinc catalyst can be isolated in 97 % yield from commercial sources (Figure 1).

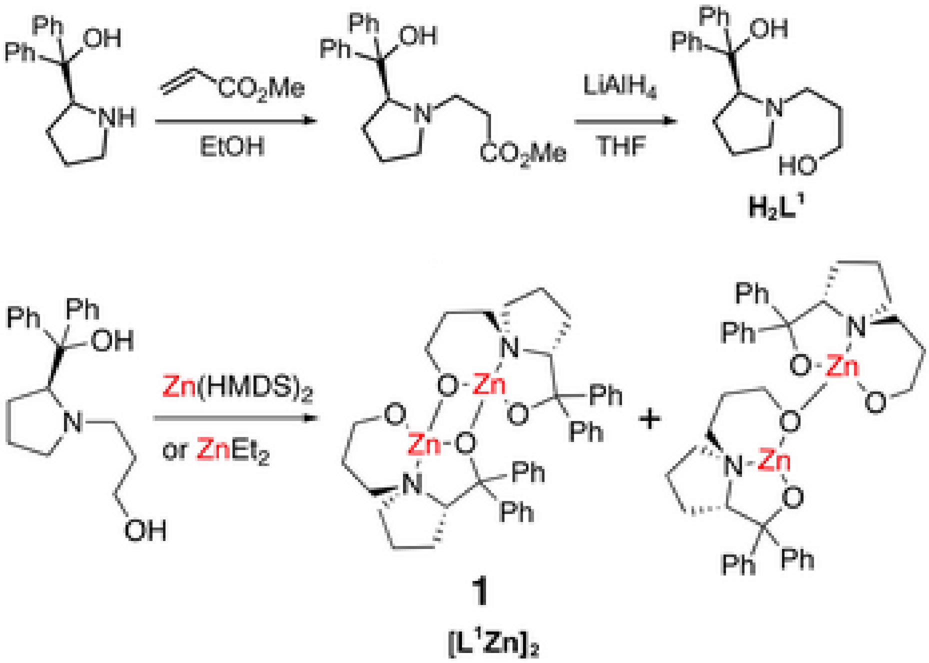

Figure 1: Synthesis of the proline derived zinc catalyst

The catalyst produces polycarbonates selectively from neat cyclohexene oxide under 1 bar of CO_2 pressure at temperatures above 50°C. At 80 °C reaction temperature, TONs of 1684 and initial TOFs up to 149 h were measured, while producing an isotactic-enriched polycarbonate with a probability of 65 % for the formation of a meso diad.

[CHO]:[cat.]	TON	TOF_{max}
1008	1684	149
1511	1461	104
2018	808	85

Table 1: TON and TOF(max) for example ratios of substrate to catalyst [CHO:cat.] . Polymerizations were performed with a pressure of 1 bar and 80°

Advantages

- the catalyst can be easily synthesized with extraordinarily high yields
- no need for highly toxic chemicals like phosgene
- polycarbonate synthesis is possible at atmospheric pressure
- high selectivity and reaction efficiency (TON /TOF)
- "green technology": CO2 binding
- nearly cost free starting material, when used in parallel to a CO2 emitting processes e.g. like PET-plastic production
- cost saving: simple reaction tanks (atmospheric pressure), less energy consumption (low pressure and temperature), lower safety costs (reduced toxicity)

Applications

The catalyst can be used for industrial synthesis of polycarbonates. The technology is especially interesting, when it established in parallel to a CO2 emitting reaction, since in this case the raw material is nearly free of cost.

Development Status

The efficiency of this proline-based catalyst is prooven in a laboratory scale, but optimization is still possible.

Patentsituation / Patent Status

We filed international PCT-IP rights and are looking for a licensing partner interested in further developing and marketing.

References

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