

POSTER PRESENTATION



Studies on the mechanism of the lactide polymerization with highly active zinc guanidine catalysts

I dos Santos Vieira¹, J Börner², U Flörke², S Herres-Pawlis^{1*}

From 6th German Conference on Chemoinformatics, GCC 2010 Goslar, Germany. 7-9 November 2010

Polylactide (PLA) is a biodegradable polyester which is able to replace petrochemical based plastics in many fields [1]. It is commonly produced by ring-opening polymerisation (ROP) of the cyclic diester lactide with metal containing initiator systems using anionic ligand systems [2].

Zinc complexes with neutral guanidine ligands have proven to be highly active initiators in the ROP of lactide [3,4]. In an integrated study combining kinetic analyses, spectroscopic measurements and DFT calculations the mechanism of the lactide polymerisation with this special catalyst class could be clarified. We could show that the polymerisation proceeds via a coordinationinsertion-mechanism.

A complete reaction coordinate diagram including enthalpies of intermediates and transition states could be compiled by B3LYP-DFT for the initiation step of the polymerisation with the initiator $[Zn(TMGqu)_2$ $(CF_3SO_3)][CF_3SO_3]$ and also for the chain propagation. The initiating step includes three transition states with 102 kJ/mol as highest activation barrier. The model for the propagation step reveals two transition states with an energy barrier not exceeding 65 kJ/mol. The results of this study demonstrate that lactide ROP proceeds not only with classical complexes using anionic ligands, but also with complexes containing neutral but highly nucleophilic guanidine ligands.

Author details

¹Anorganische Chemie II, Technical University of Dortmund, 44225 Dortmund, Germany. ²University of Paderborn, 33098 Paderborn, Germany.

* Correspondence: sonja.herres-pawlis@tu-dortmund.de

¹Anorganische Chemie II, Technical University of Dortmund, 44225 Dortmund, Germany

Full list of author information is available at the end of the article



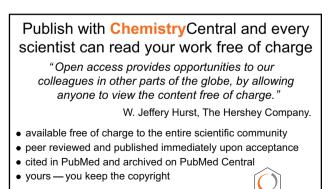
Published: 19 April 2011

References

- Gupta B, Revagade N, Hilborn J: Poly(lactic acid) fiber: An overview. Prog Polym Sci 2007, 32:455-482.
- Dechy-Cabaret O, Martin-Vaca B, Bourissou D: Controlled Ring-Opening Polymerization of Lactide and Glycolide. Chem Rev 2004, 104:6147-6176.
- Börner J, Flörke U, Huber K, Döring A, Kuckling D, Herres-Pawlis S: Lactide Polymerisation with Air-Stable and Highly Active Zinc Complexes with Guanidine-Pyridine Hybrid Ligands. Chem Eur J 2009, 15:2362-2376.
- Börner J, Herres-Pawlis S, Flörke U, Huber K: [Bis(guanidine)]zinc Complexes and Their Application in Lactide Polymerisation. Eur J Inorg Chem 2007, 5645-5651.

doi:10.1186/1758-2946-3-S1-P22

Cite this article as: dos Santos Vieira *et al.*: **Studies on the mechanism of the lactide polymerization with highly active zinc guanidine catalysts.** *Journal of Cheminformatics* 2011 **3**(Suppl 1):P22.



ChemistryCentral

Submit your manuscript here: http://www.chemistrycentral.com/manuscript/

© 2011 dos Santos Vieira et al; licensee BioMed Central Ltd. This is an open access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/2.0), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.