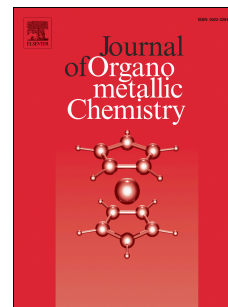


# Accepted Manuscript

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# Steric Factors on Unsymmetrical *O*-hydroxyaryl *N*-Heterocyclic Carbene Ligands Prevailing the Stabilization of Single Stereoisomer of Bis-Ligated Titanium Complexes

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## Abstract

Bis-ligated titanium(IV) metal complexes supported by bidentate unsymmetrical *o*-hydroxyaryl-substituted *N*-heterocyclic carbene ligands were synthesized and structurally identified. While the direct addition of the doubly deprotonated bulky imidazolidinium chloride salts [Dipp,<sup>4</sup>-R<sup>NHC</sup>-H]Cl (with Dipp = 2,6-diisopropylphenyl, R = H (2-hydroxyphenyl), and R = Me (2-hydroxy-4-methyl-phenyl)) with chloro-titanium precursor favors the formation of single stereoisomer corresponding to the bis-ligated titanium complexes *trans*-([κ<sup>2</sup>-C,O]-Dipp,<sup>4</sup>-R<sup>NHC</sup>)<sub>2</sub>TiCl<sub>2</sub> (R = H (2-hydroxyphenyl) for **4a<sup>H</sup>**, and R = Me (2-hydroxy-4-methyl-phenyl) for **4a<sup>Me</sup>**), the reactivity with sterically less hindered imidazolidinium chloride salts [Mes,<sup>H</sup>NHC-H]Cl and [Dep,<sup>H</sup>NHC-H]Cl as protio-ligands (with Mes = 2,4,6-trimethylphenyl and Dep = 2,6-diethylphenyl) did not lead to single stereoisomer, but rearranged into a tetradentate salophen-like complexes *cis*-([κ<sup>4</sup>-O,N,N,O]-bis(imidazolidinylidene)TiCl<sub>2</sub>) as major isomer via presumably the NHCs dimerization from bis-ligated intermediates. These results combined with topographic steric maps as well as the buried volume descriptor (%*V<sub>bur</sub>*) indicate that bidentate bulky *N*-Dipp-substituted NHC ligands offer some level of steric protection preventing the formation of other possible bis-ligated (C,O)-NHC-titanium stereoisomers and constitutional isomers.

## Keywords

Titanium; Bidentate ligand; Unsymmetrical *N*-heterocyclic carbene; Bis-ligated titanium complex; Ethylene polymerization.

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