

## OR-65

## OPTIMIZATION OF CATALYST STRUCTURE FOR ASYMMETRIC ALLYLATION-TYPE REACTIONS OF FUNCTIONALIZED TRICHLOROSILANES WITH AROMATIC ALDEHYDES

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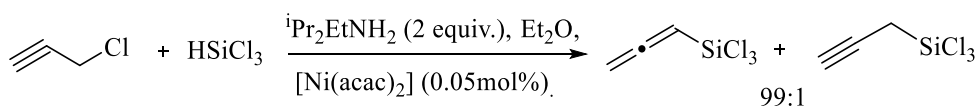
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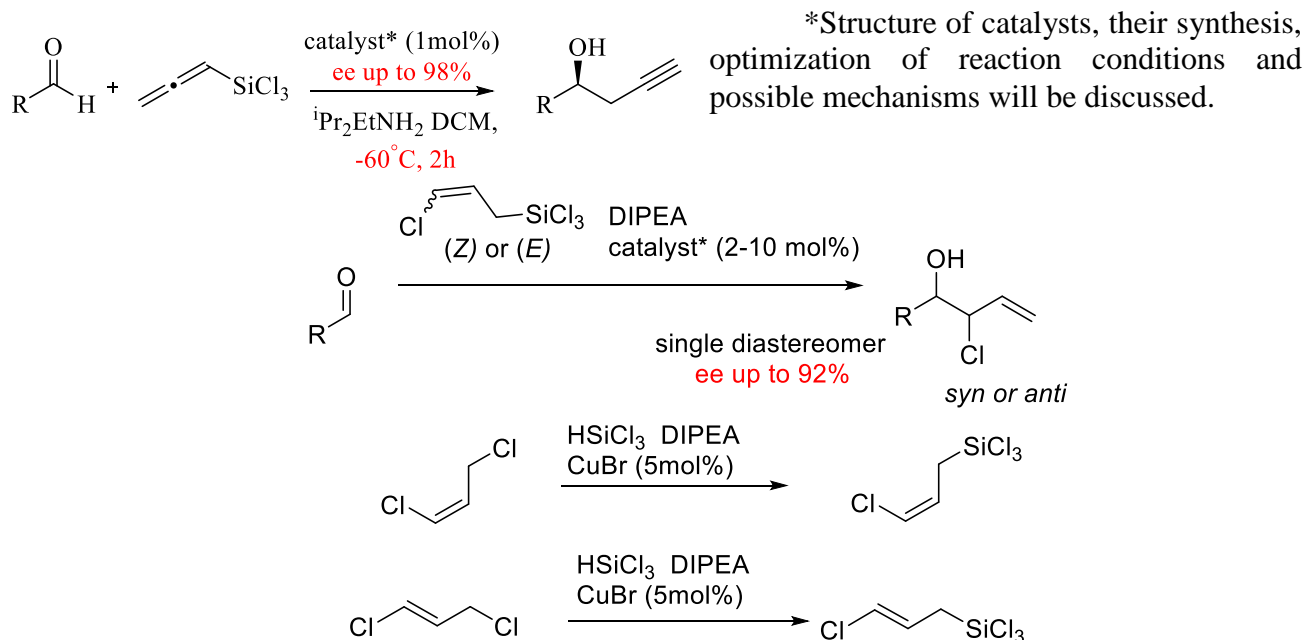
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**Abstract.** Axially-chiral bipyrindine-dioxides could be a powerful tool for asymmetric allylation-type reactions with various trichlorosilanes. In this work, we report about our recent achievements in asymmetric propargylation reactions and asymmetric allylation with  $\gamma$ -functionalized allyltrichlorosilanes with focusing on optimization of catalyst structure. The optimization is based on DFT-calculations and statistical regression analysis (using the large library of optimization experiments). In this work we've designed a series of new chiral Lewis Bases, show their excellent catalytic ability in the reaction of asymmetric propargylation of aromatic and  $\alpha$ -unsaturated aldehydes, and show their applicability in both *syn*- and *anti*-cl-allylation of aromatic aldehydes.

The reactions proceed with high level of chemo- and stereoselectivity



S. Kobayashi et al. Tetrahedron, 2006. 62(2-3): p. 496-502.



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