

A Ligand Guided Stereodivergent Alkyne Reduction Using Water as the Hydrogen Source

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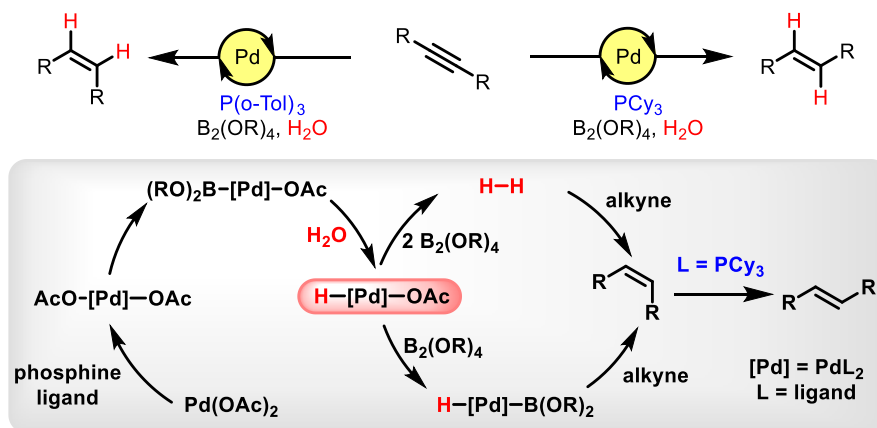
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E- and Z-alkenes, as functionality, are an integral part of many natural products/biologically interesting molecules and a key intermediate during several pertinent chemical transformations. However, their preparation is still plagued by over reduction, inefficient stereoselectivity of the resultant alkene and/or use of dangerous gaseous H₂.

Herein, we present a convenient synthesis of E- and Z-alkenes in a stereoselective manner. In contrast to traditional methods, a homogeneous method involving Pd-catalyst and a diboron reagent has been used. Most importantly, water has been employed as the H₂ source, thus circumventing the necessity of H₂ gas involved in the traditional methods. Also, by controlling the equivalents of the diboron reagent, the over-reduction of alkynes to alkanes can be avoided without compromising on the stereoselectivity.

A retro-mechanistic approach has been envisaged to understand the reactivity of diboron reagents with water. The results suggest formation of H-[Pd]-OAc as the crucial step leading to the presence of two pathways involving H-[Pd]-B(OR)₂ and molecular H₂. This approach efficiently assists in identifying pertinent intermediates responsible for the remarkable ability of diboron compounds in reducing organic substrates.



1. Rao, S; Prabhu, K.R. A Ligand Guided Stereodivergent Reduction of Alkynes Using Water as the Hydrogen Source (*manuscript submitted*).
2. Rao, S; Prabhu, K.R. A Retro-mechanistic Analysis of Diboron Mediated Alkyne Reduction Using Water as the Hydrogen Source (*manuscript submitted*).
3. Ojha, D. P.; Gadde, K.; Prabhu, K. R. Generation of Hydrogen from Water: A Pd-Catalyzed Reduction of Water Using Diboron Reagent at Ambient Conditions. *Org. Lett.* **2016**, *18*, 5062–5065.