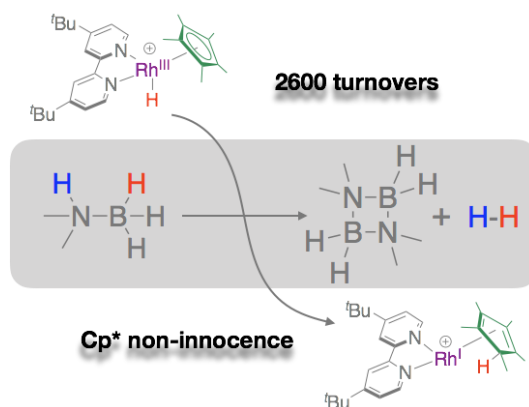


Dehydrogenation of dimethylamine-borane catalyzed by half-sandwich Ir and Rh complexes: Mechanism and the role of Cp* non-innocence

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Keywords: Amine-borane dehydrogenation, Half-sandwich Complexes, Hydrogen Storage, Cp* non-innocence

Amine-boranes are attractive candidates for hydrogen-storage. Using transition-metal catalysts, they can be dehydrogenated to produce H₂ and amino-boranes. Here we will present our recent findings on the activity of half-sandwich Rh^{III} and Ir^{III} complexes in catalytic dehydrogenation of dimethylamine-borane. These bench-stable complexes are easily synthesized from the commercially available bipyridine ligands and Cp*MCl₂-precursors (Cp*= η^5 -1,2,3,4,5-pentamethylcyclopentadienyl, M=Rh or Ir). While the Rh^{III}-analogues demonstrated turnovers of up to 2600, the Ir^{III}-complexes demonstrated very poor activity. Mechanistic inferences drawn from combined experimental and DFT investigations, and the role of non-innocent involvement of the Cp* moiety as a proton shuttle will be discussed. These findings may pave for the way for the rational design of new catalysts based on this easily accessible platform.



References:

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