

Abstract

Title: Synthesis and catalytic properties of phosphinoferrocene guanidine

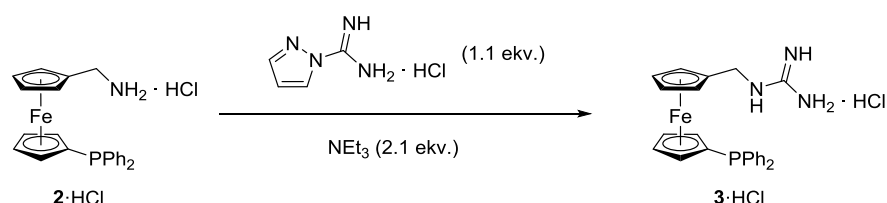
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Polar phosphine ligands proved to be useful in homogeneous and biphasic catalysis. Most of these phosphines bears anionic functional groups. On the other hand, functionalization of phosphines by cationic substituents is still quite uncommon, although these functional groups possess properties that could improve catalytic performance of the catalyst. In this regard, nitrogenous bases are particularly attractive due to their inherent basicity and the ability to enter into hydrogen bonding interactions.

This thesis describes the synthesis of a novel ferrocene-based phosphine functionalized with guanidine moiety, viz. *N*-[1'-(diphenylphosphino)ferrocenylmethyl]guanidine (**3**). This compound was obtained by direct guanylation of 1'-(diphenylphosphino)-1-(aminomethyl)ferrocene (**2**) (see scheme). Compound **3** was further used to prepare palladium complexes including the unusual zwitterionic complex [PdCl₃(**3H**)]. The molecular structures of the prepared complexes were determined by X-ray diffraction analysis.



Catalytic properties of phosphine **3** and complex [PdCl₃(**3H**)] were evaluated in Suzuki-Miyaura coupling reaction between *para*-substituted aryl bromides and bicyclic triolborates. The reaction was performed in various solvents with satisfactory results. During optimization of the reaction conditions, it was found that the reaction performed at 80 °C with 0.2% of catalyst loading affords excellent results for most of the substrates after only 3 hours.

Keywords: ferrocene; phosphine ligands; guanidine; synthesis; coordination behaviour; catalytic properties