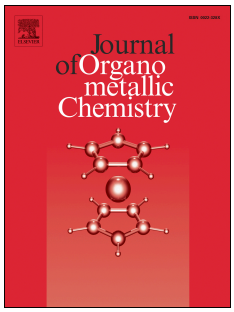
Accepted Manuscript



Synthesis and catalytic activities of 1-alkoxycarbonyl- and 1-carbamoylmethyl-5-phenyl-3-aryl-3*H*-imidazol-1-yliden-Pd(II) complexes

Meliha Çetin Korukçu, Necdet Coşkun

PII: S0022-328X(17)30030-X

DOI: 10.1016/j.jorganchem.2017.01.010

Reference: JOM 19767

To appear in: *Journal of Organometallic Chemistry*

Received Date: 9 August 2016

Revised Date: 16 January 2017

Accepted Date: 18 January 2017

Please cite this article as: M.E. Korukçu, N. Coşkun, Synthesis and catalytic activities of 1-alkoxycarbonyl- and 1-carbamoylmethyl-5-phenyl-3-aryl-3*H*-imidazol-1-yliden-Pd(II) complexes, *Journal of Organometallic Chemistry* (2017), doi: 10.1016/j.jorganchem.2017.01.010.

Synthesis and catalytic activities of 1-alkoxycarbonyl- and 1-carbamoylmethyl-5-phenyl-3-aryl-3*H*-imidazol-1-yliden-Pd(II) complexes

Meliha Çetin Korukçu, Necdet Coşkun[*]

Uludağ University, Department of Chemistry, 16059-Bursa, TURKEY

coskun@uludag.edu.tr, 90224-2941725

Abstract: 4-Phenyl-1-aryl-1*H*-imidazoles were reacted with α-haloesters and amides to give the corresponding imidazolium salts. The latter were used as starting materials for the synthesis of Pd(NHC) complexes. The catalytic activities of the newly prepared compounds were screened in a model coupling reaction. 1-Alkoxycarbonyl-5-phenyl-3-aryl-3*H*-imidazol-1-yliden-Pd(II) were shown to be better catalyst than the 1-carbamoylmethyl-5-phenyl-3-aryl-3*H*-imidazol-1-yliden-Pd(II) complexes. The catalysts were shown to be insensitive to the air oxygen and water.

Keywords: NHCs; NHC Enolates; Ag(I)-NHC complexes. Pd(II)-NHC complexes; Heck reaction.

I. INTRODUCTION

The carbon-carbon bond forming reaction between alkenes and aryl halides in the presence of a palladium catalyst has found an extensive usage following the pioneering reports of Mizoroki[1] and Heck[2] from the early 1970s.

Numerous excellent surveys on a wide variety of different aspects of the Heck reaction have been published.[3] A variety of ligands[3a] have been developed for the reaction, and it has been a key step in the total synthesis of many natural products and commercially important products.[3b,3d] The selectivity and mechanistic aspects of the carbon-carbon bond forming reactions have been thoroughly reviewed,[3c-e,4] and are still important subject of research.[5] Our laboratory has recently described the utility of isoxazolo[3,2-*a*]isoquinolines as precursors for the synthesis of stable azomethine ylides;[6a] while the adducts of acyclic nitrones were shown to undergo a cascade reaction leading to the formation of iminocarbenes.[6b] We have also reported the rearrangement of isoxazolines from the reaction of imidazoline 3-oxides with dimethyl acetylenedicarboxylate to give the corresponding 3*H*-imidazol-1-ium ylides. The reaction of the latter with $AgNO_3$ in the presence of Et_3N at room temperature provides C-2 metallated N-heterocyclic carbine enolates (Ag-NHCE) precursors such as **1** (Scheme 1).[7] The silver compounds reported so far in the formation of Ag(I)-NHC complexes are AgOAc,[8] Ag_2O[9] and Ag_2CO_3.[10] Silver N-heterocyclic carbene complexes have been important in the development of other metal–carbene systems due to facile transmetallation reactions from the silver carbenes to a wide range of other transition metals.[11-12] Palladium complexes of NHC ligands, in particular, have proved to be