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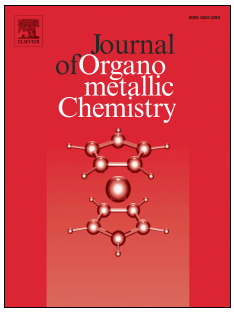

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PII: S0022-328X(18)30006-8

DOI: 10.1016/j.jorganchem.2018.01.006

Reference: JOM 20244

To appear in: *Journal of Organometallic Chemistry*

Received Date: 29 October 2017

Revised Date: 31 December 2017

Accepted Date: 5 January 2018

Please cite this article as: K. Ahmad, C.-R. Chang, J. Li, Theoretical studies on copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate under ligand-free conditions, *Journal of Organometallic Chemistry* (2018), doi: 10.1016/j.jorganchem.2018.01.006.

Theoretical Studies on Copper-catalyzed Arylation of Nitrogen Heterocycles from Benzenediazonium acetate under Ligand-Free Conditions

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Abstract

The density functional theory (DFT) method was used to investigate the mechanism of ligand-free copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate. Two possible mechanisms, single electron transfer and oxidative addition/reductive elimination reaction mechanism were investigated for two possible Cu(I) complexes in the reaction solution. Complex **1** has an acetate and a pyrazole ligand coordinated to Cu(I), and complex **2** has two pyrazole ligands coordinated to Cu(I). Both Cu(I) complexes have sufficiently low activation energy barriers for oxidative addition/reductive elimination reactions. Activation energy barrier for single electron transfer reaction is significantly higher than oxidative addition/reductive elimination reaction.

Keywords: Copper-catalyzed, C─N cross coupling, DFT, Catalytic mechanism

1. Introduction

Transition metal-catalyzed C─N bond formation is one of the most important metal catalyzed cross-coupling reactions. Products obtained by C─N coupling reactions find enormous applications in life sciences and polymer industry [1-6]. The pioneering work on copper-