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

Khalil Ahmad<sup>a,b</sup>, Chun-Ran Chang<sup>c,\*</sup> and Jun Li<sup>b,\*</sup>

<sup>a</sup>*Department of Chemistry, University of Azad Jammu and Kashmir, Muzaffarabad 13100, Pakistan*

<sup>b</sup>*Department of Chemistry and Key Laboratory of Organic Optoelectronics & Molecular Engineering of Ministry of Education, Tsinghua University, Beijing 100084, China*

<sup>c</sup>*Institute of Industrial Catalysis, School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an 710049, China*

\* Corresponding author.

*E-mail address:* changcr@mail.xjtu.edu.cn (C. R. C.) and junli@tsinghua.edu.cn (J. L.)

## 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-

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