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A Highly Efficient *N*-Heterocyclic Carbene–Copper(I) Catalyst for the Selective Synthesis of 1,2,3-Trisubstituted Triazoles †

Sarra Lasmari [1] and Sofiane Ikhlef [2,3,*]

[1] Department of Biology, Faculty Natural and Life Sciences, Ferhat Abbas University-Setif 1, Setif 19000, Algeria; saralasmari90@gmail.com
[2] Laboratoire d'Obtention de Substances Thérapeutiques (LOST), Campus Caabet Ersas, Université Constantine 1, Constantine 25000, Algeria
[3] Department of Proceeding Engineering, Institute of Sciences and Technology, Abd el Hafid Boussouf-Mila University Center, Mila 43000, Algeria
* Correspondence: s.ikhlef@centre-univ-mila.dz
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Abstract

In this study, we report the synthesis of 1,2,3-trisubstituted triazoles via a straightforward and efficient protocol. Although numerous methodologies for constructing the triazole scaffold are available in the literature, our approach offers a practical and operationally simple alternative. The reaction was catalyzed by an N-heterocyclic carbene (NHC)–Copper(I) complex, which proved to be a highly efficient catalyst. The desired triazole derivatives were obtained in excellent yields, ranging from 86% to 96%, highlighting the robustness and effectiveness of the method.

Keywords: triazole; NHC; cooper; complex

1. Introduction

N-Heterocyclic carbenes (NHCs) have established themselves as one of the most versatile and widely utilized ligand families in organometallic chemistry, particularly in the field of homogeneous catalysis [1]. Their exceptional ability to form strong and stable bonds with transition metals has facilitated the development of a wide range of metal–NHC complexes, which have found valuable applications not only in catalysis but also in medicinal chemistry and, more recently, in materials science [2]. The increasing interest in NHC-based systems has spurred significant efforts toward the design of sustainable, efficient, and practical synthetic routes for their preparation, further expanding their accessibility and utility in modern chemical research [3,4].

2. Synthesis

The catalytic activity of the (Cu–NHC) complexes was evaluated using the 1,3-dipolar cycloaddition between phenylacetylene and benzyl azide as a model reaction to optimize the reaction conditions (Table 1). A solvent screening was initially performed, revealing that ethanol was the most suitable medium. In contrast, significantly lower yields were obtained when water, toluene, or dichloromethane were used, likely due to the limited solubility of the NHC–Cu(I) catalysts in these solvents (Table 1, entries 1, 2, and 5).

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Table 1. Optimization of the reaction.

Entry	Cat. (mol%)	Solvent	Time	Isolated Yield
1	2 mole %	CH_2Cl_2	8 h	40
2	2 mole %	Toluene	8 h	52
3	2 mole %	MeOH	8 h	85
4	2 mole %	EtOH	8 h	96
5	2 mole %	H_2O	8 h	trace

3. Results and Discussion

To further assess the synthetic utility of the (Cu–NHC) complex, its catalytic efficiency was explored in the reaction of benzyl halides with phenylacetylene. The study was then extended to evaluate the reactivity of phenylacetylene with a diverse range of alkyl and aryl halides. In all cases, the reactions proceeded efficiently, furnishing the corresponding 1,2,3-disubstituted triazoles as single regioisomers in excellent yields. A more comprehensive investigation was subsequently carried out in ethanol, employing various alkyl halides to synthesize both N-aryl and *N*-alkyl triazole derivatives. The crude products were purified by silica gel column chromatography, affording pure compounds in isolated yields ranging from 86% to 96% (Table 2).

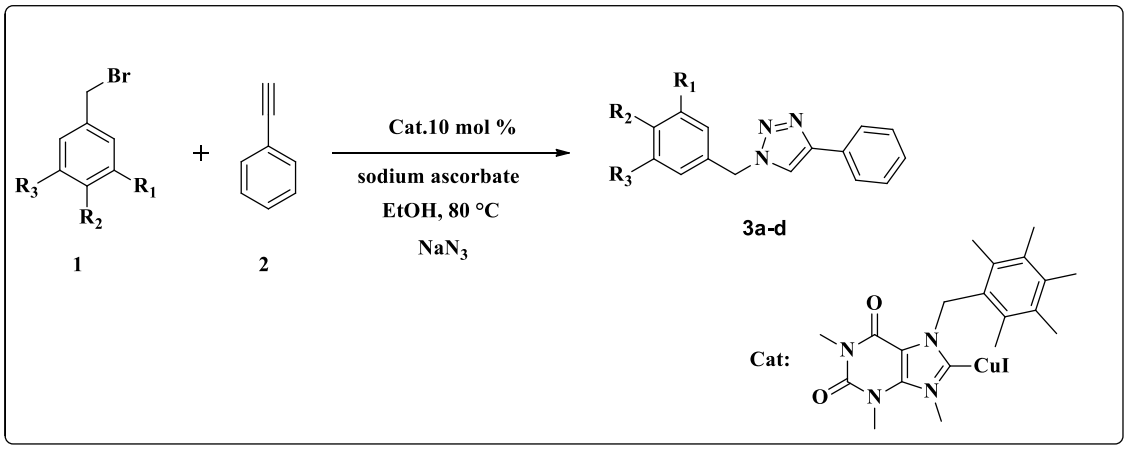

Figure 1. General route to synthesize 1,2,3 Triazoles.

Table 2. One-Pot Three-Component Click Reaction for Compounds 4a–d.

Entry	R_1	R_2	R_3	Products	Yields
1	H	H	H	3a	**94**
2	H	*t*bu-	H	3b	**96**
3	CH_3	H	CH_3	3c	**88**
4	H	CH_3	H	3d	**86**

4. Conclusions

In conclusion, the NHC–Cu catalyst demonstrates excellent efficiency in the synthesis of 1,2,3-substituted triazoles from phenylacetylene and various alkyl halides. The reactions proceed smoothly under mild conditions, consistently affording products with high purity and good to excellent yields.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/doi/s1.

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