

# Silver(I)-Catalyzed Azide-Alkyne Cycloaddition Reaction in Water. Scope and Mechanistic Aspects

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## Abstract

A combined experimental work and molecular electron density theory (MEDT) analysis was performed to reveal the strict click of 1,2,3-triazole derivatives by Ag(I)-catalyzed azide-alkyne cycloaddition (AgAAC) reaction and its corresponding mechanistic pathway. Such straightforward protocol for the click formation of 1,4-disubstituted-1,2,3-triazoles makes use of AgCl as catalyst in water as solvent under ambient conditions, with excellent yields and simple experimental work-up. MEDT study was performed by using DFT calculations at the B3LYP/6-31G(d,p) (LANL2DZ for Ag) level in order to understand the observed regioselectivity in AgAAC reactions, and to delineate the number of silver(I) species and their roles in this clickable 1,2,3-triazole formation. The comparison of the mononuclear Ag(I)-acetylide and binuclear Ag(I)-acetylide in the AgAAC reaction paths concerning the AgAAC reactions, shows that the values of the energy barriers for the binuclear processes are smaller than that of the mononuclear one. The intramolecular nature of these AgAAC reactions accounts for the regioselective formation of the 1,4-regioisomeric triazole derivatives. The ionic nature of the starting metallated species is revealed for the first time, ruling out any covalent interaction involving the silver(I) complexes throughout the reaction as supported by the ELF topological analysis of the electronic structure of the stationary points, reaffirming the zw-type mechanism of the AgAAC reactions.

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