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Synthesis, characterization and computational study of CuI nanoparticles immobilized on modified poly (styrene-co-maleic anhydride) as a green, efficient and recyclable heterogeneous catalyst in the synthesis of 1,4-disubstituted 1,2,3-triazoles via click reaction

[Majid M. Heravi](#)¹, Fatemeh Ebrahimpour-Malamir, Tayebah Hosseinnnejad, Razieh Mirsafaei

¹ Department of Chemistry, Faculty of Physics & Chemistry Alzahra University, Vanak, Tehran, Iran.

Abstract

Poly (styrene-co-maleic anhydride) (SMA) was modified by reaction with 4-amino-2-methyl-10H-thiene [2,3-b][1,5]-benzodiazepine (ATD) hydrochloride, providing an imide with the appropriate sites for the coordination of Cu(I) ions. This modified SMA was reacted with CuI to obtain immobilized Cu(I) NPs. This Cu(I) NPs (CuI/SMI-TD) was fully characterized by conventional techniques such as FT-IR, NMR, SEM, TEM, EDAX and ICP-AES analysis. The SEM and TEM images clearly showed CuI NPs as spherical shapes and the size of particles is 30-60 nm. Moreover, a quantitative description for experimental features of CuI/SMI-TD was presented via computational assessment for the interactions between copper metal ions and coordination sites of SMI-TD ligand. The catalytic activity of this new catalyst was examined in the regioselective synthesis of 1,4-disubstituted-1,2,3 triazoles in a classical copper-catalyzed reaction a so-called click reaction. The catalyst showed highly efficient catalytic activity, excellent reusability, high yield and more importantly excellent, regioselectivity. The catalyst was recoverable through simple filtration and can be reused at least five times without significant loss of catalytic activity. The heterogeneous nature of the catalyst was confirmed based on the hot filtration test and ICP-AES analysis.

Keywords: 1,2,3-Triazoles, click reaction, density functional theory, heterogeneous copper nanocatalyst, poly(styrene-co-maleic anhydride) (SMA), quantum theory of atoms in molecules, Atomic emission spectroscopy, Catalysts, Computation theory, Copper, Maleic anhydride, Metal ions, Metals, Quantum theory, Regioselectivity, Reusability, Styrene, Synthesis (chemical), Nano-catalyst.

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