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Cu@furfural imine-decorated halloysite as an efficient heterogeneous catalyst for promoting ultrasonic-assisted A3 and KA2 coupling reactions: A combination of experimental and computational study

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Abstract

Halloysite nanoclays (HNTs) were functionalized with (3-chloropropyl) trimethoxysilan and subsequently reacted with thiosemicarbazide and furfural to furnish furfural imine functionalized HNTs, which could serve as an efficient support for immobilization of copper species. The obtained catalyst, Cu@HNTs-T-F, was fully characterized using SEM/EDX, FTIR, ICP, TGA, XRD and BET. To present a theoretical description of the experimental features of the Cu@HNTs-T-F nano catalyst, we modeled and computationally assessed two coordination modes between copper acetate and the HNTs-T-F ligand in the gas and solution phases. In this line, the mathematical properties of electron density functions were calculated and analyzed topologically via density functional theory (DFT) and quantum theory of atoms in molecules (QTAIM) approaches. Encouraged by our computational results, the catalytic activity of this new catalyst was studied for A3 and KA2 coupling reactions of aldehydes or ketones, phenyl acetylene and amines under green, ultrasonic-assisted conditions. The results established that the catalyst could promote the reaction to furnish the corresponding propargylamine derivatives in high yields in very short reaction times. Studying the reusability of the catalyst confirmed that the catalyst could be recovered and reused up to four times with only a negligible loss of the catalytic activity, indicating the efficiency of the functionalized HNTs on anchoring the copper species. ICP-AES analysis established very low leaching of copper species upon reuse. This observation was attributed to the interactions of heteroatoms in the functionalized HNTs with copper. Moreover, the results confirmed the heterogeneous nature of the catalysis.

Keywords: aldehyde, amine, copper acetate, Article, furfural, imine, ketone, thiosemicarbazide, adsorption, density functional theory, desorption, immobilization, molecular interaction, nanocatalyst, polymerization, priority journal, quantum theory, reaction time, surface area, surface property, synthesis, thermography