A new Schiff-base 2-benzoylpyridine Complex Copper on boehmite nanoparticles as a recoverable catalyst for the homoselective synthesis of 5-substituted tetrazoles

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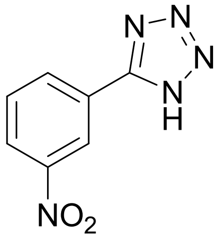
Abstract

In this research, boehmite nanoparticles (B-NPs) were prepared by a simple progress and then its surface was modified by 3-aminopropyl)triethoxysilane (3-APTES). The modified B-NPs (3-APTES@B-NPs) were functionalized by 2-benzoylpyridine Schiff-base ligand toward immobilization of Schiff-base 2-benzoylpyridine ligand on the 3-APTES@B-NPs's surface (2BP-Schiff-base@B-NPs). Finally, copper ions were coordinated with supported Schiff-base ligand on B-NPs toward formation of final catalyst (Cu-2BP-Schiff-base@B-NPs). The prepared Cu-2BP-Schiff-base@B-NPs was characterized by FT-IR, BET, XRD, SEM, AAS, TGA, EDX and mapping. In the next part, Cu-2BP-Schiff-base@B-NPs was applied as a homoselective and recyclable catalyst for the synthesis of a diverse range of 5-substituted tetrazoles in PEG-400 as a green solvent. The main benefits of this protocol are high homoselectivity attribute, short reaction times, high product yields and TOF values, and more addition the catalyst's ability to be recycled at least four times without significant losing catalytic efficiency.

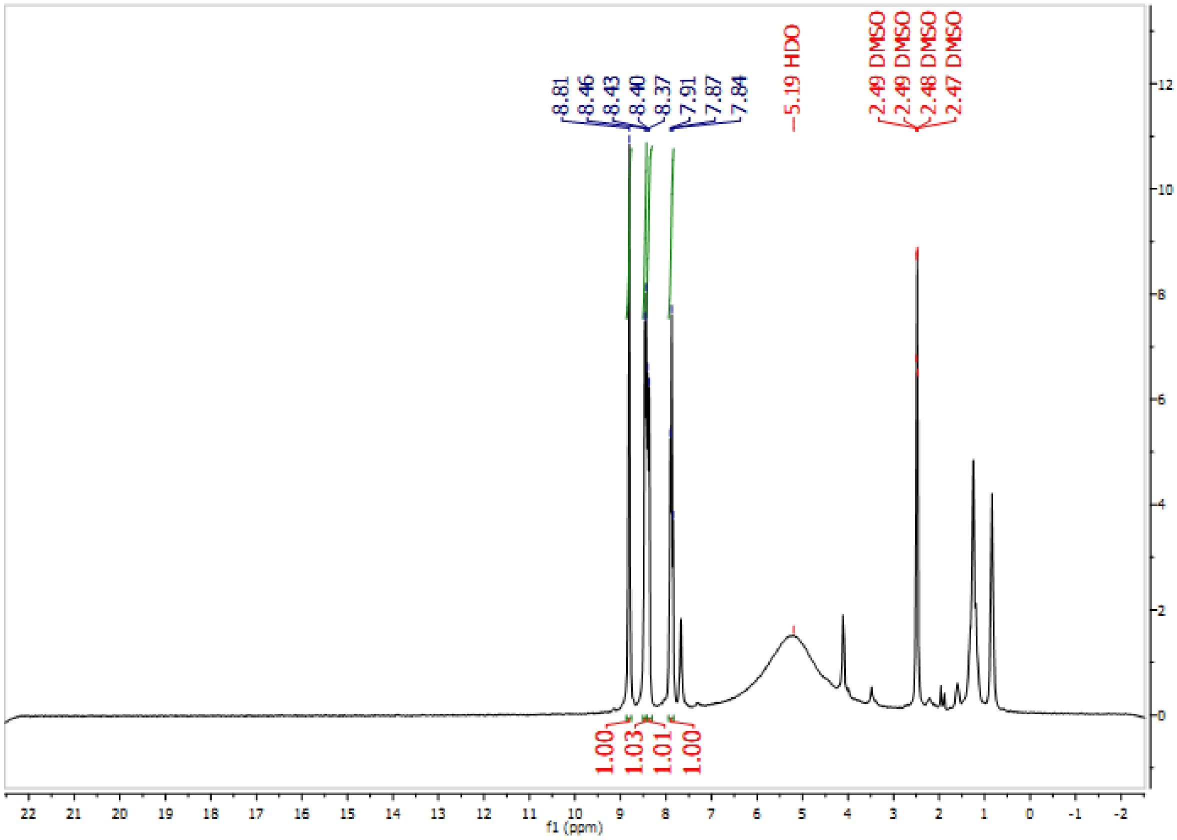
Keywords: Schiff-base ligand, copper complex; boehmite nanoparticles, homoselective catalyst, 5-substituted tetrazoles

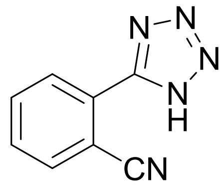
^{1}H NMR spectral data



5-(3-nitrophenyl)-1H-tetrazole

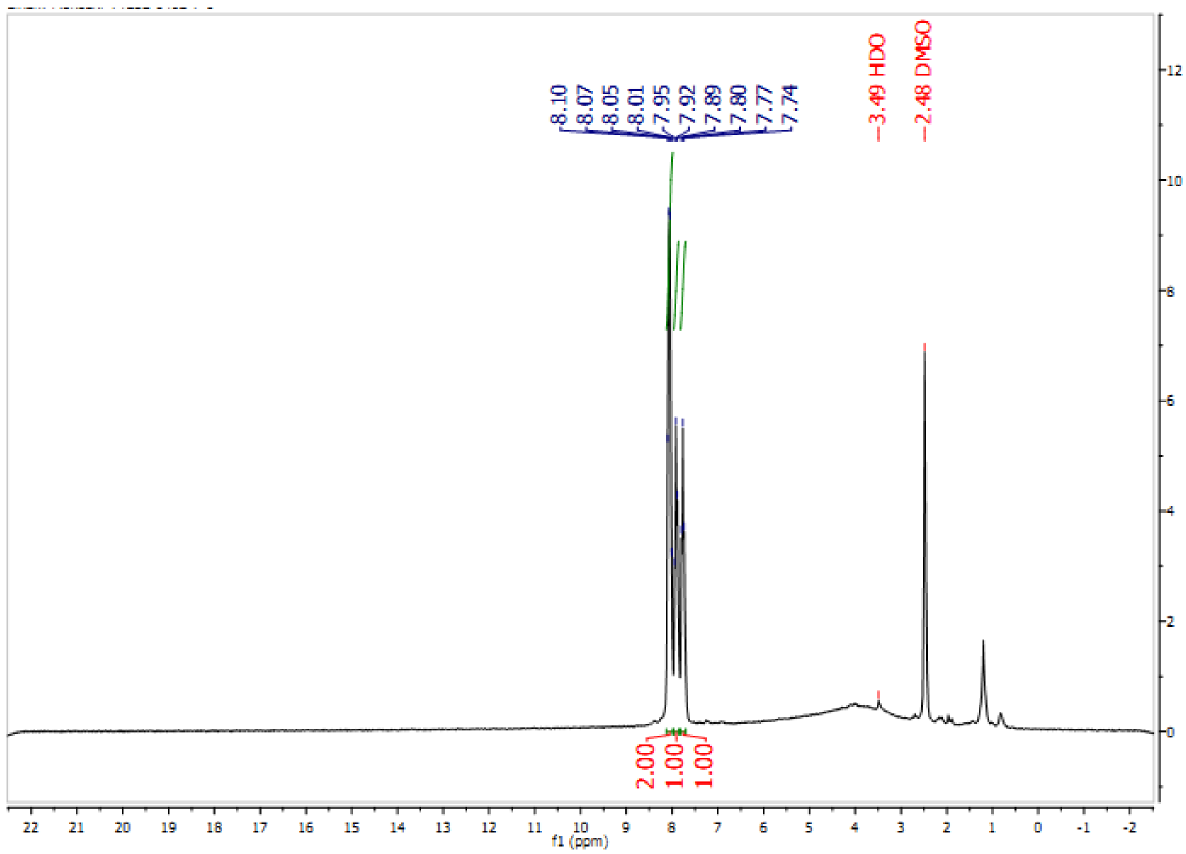
^{1}H NMR (400 MHz, DMSO-d6): δ_H= 8.81 (s, 1H), 8.46-8.43 (d, *J*= 12 Hz, 1H), 8.40-8.37 (d, *J*= 12 Hz, 1H), 7.91-7.84 (t, *J*= 12 Hz, 1H) ppm.

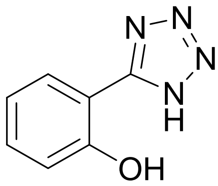




2-(1H-tetrazol-5-yl)benzonitrile

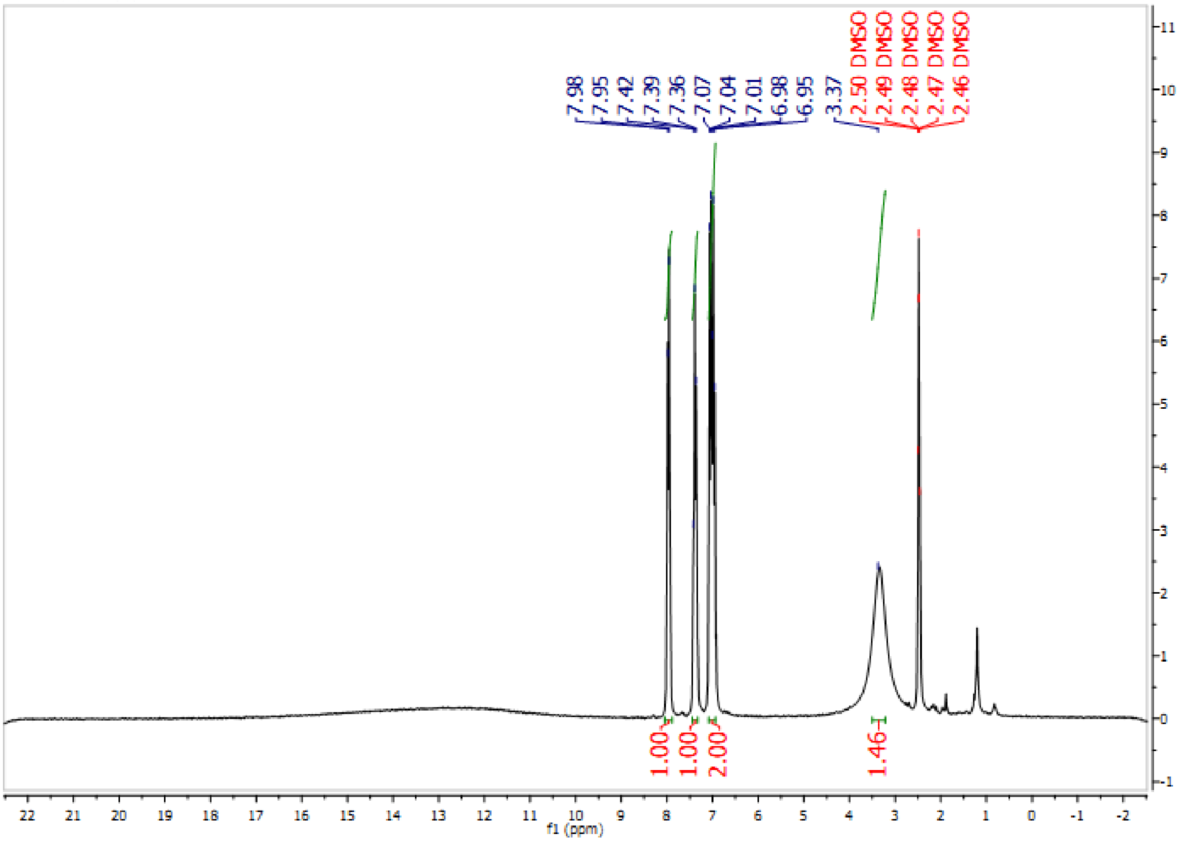
^{1}H NMR (400 MHz, DMSO-d6): δ_H= 8.10-8.05 (m, 2H), 7.95-7.89 (t, *J*= 12 Hz, 1H), 7.80-7.74 (t, *J*= 12 Hz, 1H) ppm.

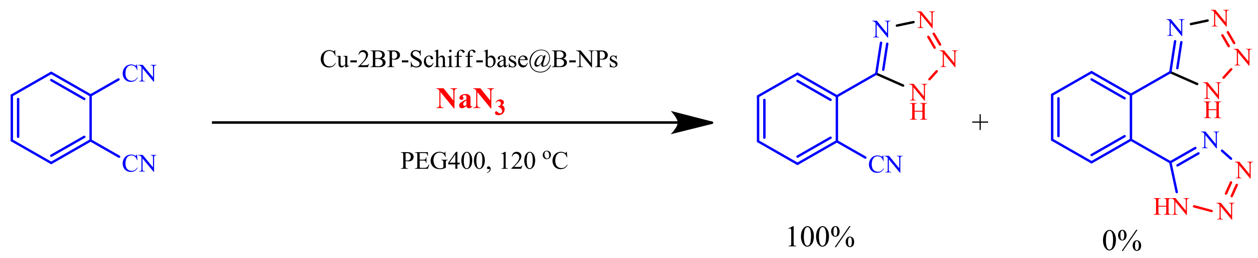




2-(1H-tetrazol-5-yl)phenol

^{1}H NMR (400 MHz, DMSO-d6): δ_H= 7.98-7.95 (d, *J*= 12 Hz, 1H), 7.42-7.36 (t, *J*= 12 Hz, 1H), 7.07-6.95 (m, 2H), 3.37 (br, 1H) ppm.





Scheme S1. Homoselectivity of Cu-2BP-Schiff-base@B-NPs in the synthesis of tetrazoles.

Table S1. Comparison of catalytic efficiency of Cu-2BP-Schiff-base@B-NPs in the model reaction of synthesis of 5-phenyl-1H-tetrazole.

Entry	Catalyst	Time (h)	Yield (%)	Reference
1	CoY Zeolite	14	95	1
2	Cu–Zn alloy nanopowder	10	94	2
3	$B(C_6F_5)_3$	8	95	3
4	Fe_3O_4@SiO_2/Salen Cu(II)	7	81.1	4
5	Fe_3O_4/ZnS HNSs	24	86	5
6	Mesoporous ZnS	36	98	6
7	$CuFe_2O_4$	12	90	7
8	Nano ZnO/Co_3O_4	12	98	8
9	Fe_3O_4@boehmite NPs	4	97	9
10	Ni-MP$(AMP)_2$@Fe-biochar	4	97	10
11	Cu-2BP-Schiff-base@B-NPs	2	95	This work

[a]Isolated yield

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