Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018 Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Synthesis and Characterization of Co₃O₄ Immobilized on Dipeptide-Functionalized Silica-Coated Magnetite Nanoparticles: As a Catalyst for **Selective Aerobic Oxidation of Alcohols**

Mohammad Mehdi Khodaei,^[a,b]* Mahsa Dehghan^[b]

^[a] Department of Organic Chemistry, Razi University, Kermanshah 67149-67346, Iran.

^[b] Nanoscience & Nanotechnology Research Center (NNRC), Razi University, Kermanshah 67149-

67346, Iran

Table of Contents:

- 1. FE-SEM and TEM measurements of the Co₃O₄@SCM-UIL catalyst
- 2. GC-mass analysis for oxidation of benzyl alcohol to benzaldehyde at optimum conditions

3. Characterization of pyridine-contained dipeptide (N-benzyl-N-(2-(cyclohexylamino)-2-oxo-1-(pyridin-3-yl)ethyl)benzamide)

- 3.1. ¹H NMR spectrum
- 3.2. ¹³C NMR spectrum
- 3.3. FT-IR spectrum

1. FE-SEM and TEM measurements of the Co₃O₄@SCM-UIL catalyst

FE-SEM, Mapping and EDX analyses were performed on a ZEISS SIGMA VP-500 instrument. TEM analysis was performed using a ZEISS-EM 10C at an acceleration voltage of 100 kV. The sample was sputtered by gold to avoid undesirable electron charging. As shown in Fig. 1Sa and 1Sb, the SCM-Cl particles show semi-spherical morphology with degrees of aggregation between particles. The average diameters of these particles are 35-57 nm. In the case of Co₃O₄@SCM-UIL (Fig. 1Sc, 1Sd and 1Sf), the diameters of the nanoparticles have not changed in comparison with the SCM-Cl particles but low degrees of aggregation are observed. By EDXS analysis, cobalt along with oxygen was detected in Co₃O₄@SCM-UIL particles (Fig. 1Se), suggesting that they consist of Co₃O₄. In the mapping technique of the catalyst, in addition to presence of the desired elements, uniform dispersion of the Co₃O₄ NPs onto the functionalized magnetic NPs is also observed (Fig. 1Sg). In the TEM images of SCM-Cl in Fig. 1Sh, 1Si and 1Sj, the core-shell structure with Fe₃O₄ cores in size range of 8 to 10 nm is observed. It is seen the same structure for the SCM-UIL NPs in Fig. 1Sn before immobilization of Co₃O₄ NPs but after immobilization of Co₃O₄ NPs (Fig. 1Sk, 1Sl, 1Sm and 1So), two types of small particles are visible. Particles with average sizes of 8-10 nm (darker black spots) are attributed to the Fe₃O₄ NPs and particles lower than 5 nm (brighter black spots) related to Co₃O₄ NPs. These small particles (lower than 5 nm) agree very well with the XRD pattern showing only very weak signals of Co₃O₄ (Fig. 2c).













Figure 1S. The FE-SEM images of SCM-Cl (a and b) and $Co_3O_4@SCM$ -UIL (c, d and e), EDX analysis of $Co_3O_4@SCM$ -UIL (f), mapping analysis of $Co_3O_4@SCM$ -UIL (g), and TEM images of SCM-Cl (h, i and j), $Co_3O_4@SCM$ -UIL (k, l, m and o) and SCM-UIL (n).

2. GC-mass analysis for oxidation of benzyl alcohol to benzaldehyde at optimum conditions

The products were analyzed by a Varian 3900 GC. Based on obtained results from GC-mass analysis for oxidation reaction of benzyl alcohol in acetonitrile as solvent under O_2 blowing at 70 ° C in the presence of $Co_3O_4@SCM$ -UIL as catalyst and undecane was used as an internal standard. The main product was benzaldehyde (76%) and 14% of benzoic acid as a by-product produced, while 10% of benzyl alcohol was not reacted. The results are shown in Fig. 2S.





b



Figure 2S. The GC analysis for the product of benzyl alcohol oxidation (a), the mass spectra of benzaldehyde (b), benzyl alcohol (c) and benzoic acid (d).

3. Characterization of pyridine-contained dipeptide (N-benzyl-N-(2-(cyclohexylamino)-2-oxo-1-(pyridin-3-yl)ethyl)benzamide)

3.1. ¹H NMR spectrum



3.2. ¹³C NMR spectrum



3.3. FT-IR spectrum

