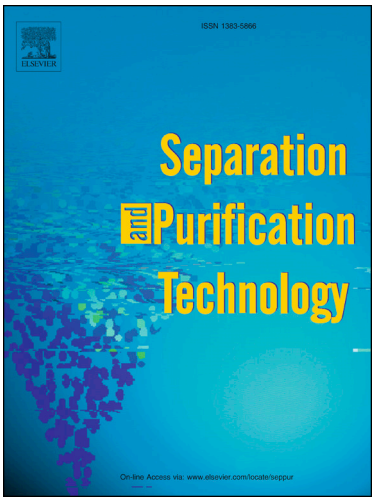

Synthesis, characterization and application of Fe_3O_4@SiO_2 nanoparticles supported palladium(II) complex as a magnetically catalyst for the reduction of 2,4-dinitrophenylhydrazine, 4-nitrophenol and chromium(VI): A combined theoretical (DFT) and experimental study

Mahmoud Nasrollahzadeh, Zahra Issaabadi, Reza Safari

PII: S1383-5866(18)31833-1
DOI: https://doi.org/10.1016/j.seppur.2018.07.022
Reference: SEPPUR 14753

To appear in: *Separation and Purification Technology*

Received Date: 28 May 2018
Revised Date: 3 July 2018
Accepted Date: 10 July 2018

Please cite this article as: M. Nasrollahzadeh, Z. Issaabadi, R. Safari, Synthesis, characterization and application of Fe_3O_4@SiO_2 nanoparticles supported palladium(II) complex as a magnetically catalyst for the reduction of 2,4-dinitrophenylhydrazine, 4-nitrophenol and chromium(VI): A combined theoretical (DFT) and experimental study, *Separation and Purification Technology* (2018), doi: https://doi.org/10.1016/j.seppur.2018.07.022

Synthesis, characterization and application of Fe_3O_4@SiO_2 nanoparticles supported palladium(II) complex as a magnetically catalyst for the reduction of 2,4-dinitrophenylhydrazine, 4-nitrophenol and chromium(VI): A combined theoretical (DFT) and experimental study

Mahmoud Nasrollahzadeh,* Zahra Issaabadi, Reza Safari

Department of Chemistry, Faculty of Science, University of Qom, Qom 3716146611, Iran

ABSTRACT

In the present work, a new catalytic system based on palladium(II)-tetrazole complex immobilized on silica-coated Fe_3O_4 (Fe_3O_4@SiO_2) nanoparticles ([Fe_3O_4@SiO_2-Tet-Pd(II)]) is introduced. In the first stage, the geometry optimization and calculations of structural and electronic properties of molecular system 5-phenyl-1*H*-tetrazole-Pd (II) complex have been carried out at UB3LYP/6-31G*/LANL2DZ level of theory. Then, the [Fe_3O_4@SiO_2-Tet-Pd(II)] was prepared via immobilizing 5-phenyl-1*H*-tetrazole as a suitable ligand on the surface of Fe_3O_4@SiO_2 as a support. The [Fe_3O_4@SiO_2-Tet-Pd(II)] as a novel magnetically catalyst was characterized by XRD, FT-IR, FE-SEM, EDS, TG-DTA and VSM. This heterogeneous catalytic system demonstrated high activity in the reduction of 2,4-dinitrophenylhydrazine (2,4-DNPH), 4-nitrophenol (4-NP) and Cr(VI) in the present of $NaBH_4$ as the reduction agent at room temperature and was reusable five times with no obvious decrease of catalytic activity.

Keywords: Palladium complex; Theoretical studies; [Fe_3O_4@SiO_2-Tet-Pd(II)]; Magnetic nanocatalyst; Reduction; Cr(VI); Nitro compounds

1. Introduction

Recently, metal complexes have attracted much attention in different areas such as biotechnology, materials science and modern chemistry [1]. In general, the metal complex has a central metal atom or ion and one or more ligands.

*Corresponding author. Tel.: +98 25 32850953; Fax: +98 25 32103595.

E-mail address: mahmoudnasr81@gmail.com (M. Nasrollahzadeh).