Accepted Manuscript

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PII: DOI: Reference:	S1386-1425(18)30394-9 doi:10.1016/j.saa.2018.05.004 SAA 16027
To appear in:	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
Received date: Revised date: Accepted date:	22 November 2017 7 April 2018 1 May 2018

Please cite this article as: Mehdi Zamani, Ali Moradi Delfani, Morteza Jabbari , Scavenging performance and antioxidant activity of γ -alumina nanoparticles towards DPPH free radical: Spectroscopic and DFT-D studies. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:10.1016/j.saa.2018.05.004

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Scavenging performance and antioxidant activity of γ-alumina nanoparticles

towards DPPH free radical: Spectroscopic and DFT-D studies

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ABSTRACT

The radical scavenging performance and antioxidant activity of γ -alumina nanoparticles towards 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical were investigated by spectroscopic and computational methods. The radical scavenging ability of γ -alumina nanoparticles in the media with different polarity (i.e. *i*-propanol and *n*-hexane) was evaluated by measuring the DPPH absorbance in UV-Vis absorption spectra. The structure and morphology of γ -alumina nanoparticles before and after adsorption of DPPH were studied using XRD, FT-IR and UV-Vis spectroscopic techniques. The adsorption of DPPH free radical on the clean and hydrated γ -alumina (1 1 0) surface was examined by dispersion corrected density functional theory (DFT-D) and natural bond orbital (NBO) calculations. Also, time-dependent density functional theory (TD-DFT) was used to predict the absorption spectra. The adsorption was occurred through the interaction of radical nitrogen N' and NO₂ groups of DPPH with the acidic and basic sites of γ -alumina surface. The high potential for the adsorption of DPPH radical on γ -alumina nanoparticles was investigated. Interaction of DPPH with Brønsted and Lewis acidic sites of γ -alumina was more favored than Brønsted basic sites. The following order for the adsorption of DPPH over the different active sites of γ -alumina was predicted: Brønsted base < Lewis acid < Brønsted acid. These results are of great significance for the environmental application of γ -alumina nanoparticles in order to remove free radicals.

Keywords: γ-Alumina, DPPH, Antioxidant, Radical scavenger, Adsorption, DFT

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