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Facile green synthesis of samarium sesquioxide nanoparticle as a quencher for biologically active imidazole analogues: Computational and experimental insights

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ABSTRACT

A green synthetic approach for the synthesis of nanoparticles (NPs) is important to maintain sustainable development. Here we report the synthesis of samarium sesquioxide (Sm_2O_3) nanoparticles using an eco-friendly and unconventional method that utilizes pineapple peel extract as a reducing agent and stabilizer. The synthesized Sm_2O_3 NP was characterized using X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) techniques, scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The density function theory (DFT) calculation was utilized to examine the various molecular properties of the biological potent imidazole analogues, namely 4-(4-(4-nitrophenyl)-5-(4-(trifluoromethyl)phenyl)-1H-imidazol-2-yl)phenol (NTIP) and 4-(4-(4-nitrophenyl)-5-(4-(trifluoromethyl)phenyl)-1H-imidazol-2-yl)aniline (NTIA) at 6–31 G basis set. The predicted HOMO and LUMO energies revealed that the molecules were chemically active and have a tendency for molecular interactions. The solvatochromic fluorescence behavior of NTIP and NTIA has been studied in different solvents ranging from non-polar to polar. Spectroscopic methods such as absorption and fluorescence methods were used to analyze the interaction of Sm_2O_3 nanoparticles with NTIP and NTIA. Association strength of these compounds with nanoparticle was estimated and observed that the NTIP has a stronger association with Sm_2O_3 nanoparticle. Stern-Volmer plots were observed to be linear except for the compounds. The estimation of the quenching rate parameter and fluorescence lifetime affirmed the occurrence of a static quenching mechanism. From the fluorescence data, the binding constants and the number of the binding sites were estimated and the quenching mechanism was driven by the electron transfer process.

1. Introduction

Rare earth metal oxides have been used in a wide range of applications, including sensors, electronic devices, and catalysis. Furthermore, because of their small size, quantum size, tunneling, and interfacial effects, rare earth oxides are of particular interest [1,2]. Among rare earth oxides, samarium oxide nanoparticles are one of the most extensively used rare earth metal oxide nanomaterials in a variety of fields, including nanoelectronics, semiconductor glasses, solar cells, sensors and resistance random access memories [3–5]. Due to its specific technological importance, there has been a great interest in finding less hazardous and economical synthetic methods. Sm_2O_3 nanoparticles, nanorods, nanofibers and nanowires have been synthesized using different physical and chemical approaches like thermal decomposition, laser-induced deposition, sputtering, hydrogen-plasma assisted growth, sol-gel, hy-

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