



Dinuclear uranyl coordination compound: Structural investigations and selective fluorescence sensing properties

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ABSTRACT

The presence of Pb(II) ions and antibiotics in water beyond the permissible limits are among the leading factors causing water pollution. Therefore, their identification is quite necessary. In this article, we are concerned with a new dinuclear uranyl coordination compound holding a 1,3-bis(2-oxy-3-methoxybenzylidene)propan-2-olate moiety, in which each uranyl ion is seven coordinated. To obtain additional insights into the structure, DFT analyses were performed. Furthermore, Hirshfeld surface analysis was also recorded to determine the various intermolecular interactions in the studied coordination compound. The studied dinuclear uranyl coordination compound exhibited excellent fluorescence properties in water making it a promising candidate for sensing Pb(II) ions and antibiotics. The results suggest the studied compound has a high sensitivity for Pb(II) ions and the antibiotic Cefuroxime, with detection limits of 44.7 and 175 nM, respectively.

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1. Introduction

Uranium, isolated from pitchblende as uranium oxide, is a very important element used in nuclear fuel, weapons and fission power plants [1,2]. In addition, uranium has a variety of oxidation states. However, +VI is the only oxidation state stable under aerobic conditions, in the form of the uranyl(VI) cation UO_2^{2+} [3–5]. Furthermore, uranyl ions have played an important role in the processing of uranium ore, nuclear fuel and nuclear wastes [6]. It is worth mentioning that the hexavalent diuranyl ion, responsible for diverse structures of uranium, is the most important functional unit in the chemistry of uranium [6–10]. In addition, the divalent uranyl ion is highly stable and possesses two covalently bonded and linearly arranged terminal oxygen atoms that promote an equatorial arrangement for ligand coordination in its complexes [11]. The inertness of uranium-oxygen double bonds ($\text{U}=\text{O}$) is thought to be due to the unique confluence of electronic effects that lead to the formation of strong and unreactive $\text{U}=\text{O}$ bonds [1]. Furthermore, in the equatorial plane the uranyl ion can coordinate with four to six additional donor atoms lying perpendicular to

the axis of the uranium ion to form various geometric configurations [9,11–14]. Over the years, uranyl complexes have been the focus of growing interest in broad areas of research, including photochemistry, gas sorption, ion-exchange, catalysis, photocatalysis, proton conductivity and nuclear power, as well as in the extraction of uranium from the sea and its removal from the environment and the human body [10,15–20]. There are several reports of Schiff bases and their applications in the areas of catalysis, analytical chemistry (detecting and removing metal ions), fluorescence and quantitative analysis [21–23], biological activity and the evaluation of notable structural features [24]. Schiff base ligands, with multiple N and O donors, have always been a suitable choice for constructing versatile multinuclear architectures because of their rich coordination capacity, low cost and straightforward synthesis [25–29]. Here, we report a new and rare dinuclear uranyl(VI) coordination compound from a multisite Schiff base ligand, 1,3-bis(2-oxy-3-methoxybenzylidene)propan-2-olate [30]. This is the first report of the usage of 1,3-bis(2-oxy-3-methoxybenzylidene)propan-2-olate or its analogs in the preparation of a dinuclear uranyl(VI) coordination compound. Earlier reports of this ligand or its analogs reveal its usage in the synthesis of multinuclear complexes. The synthesized dinuclear uranyl(VI) coordination compound was investigated by various spectroscopic studies,

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